



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 111586

TO: Michael Lavilla
Location: REM 5e79
Thursday, January 08, 2004
Art Unit: 1775
Phone: 571-272-1539
Serial Number: 09 / 700821

From: Jan Delaval
Location: Biotech-Chem Library
Remsen Building – 1A51
Phone: 571-272-2504

jan.delaval@uspto.gov

Search Notes

10/6/2000

=> fil reg

FILE 'REGISTRY' ENTERED AT 07:55:34 ON 08 JAN 2004

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STRUCTURE FILE UPDATES: 6 JAN 2004 HIGHEST RN 634878-43-6

DICTIONARY FILE UPDATES: 6 JAN 2004 HIGHEST RN 634878-43-6

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

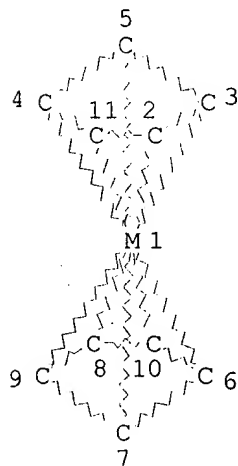
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 116

L7 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 11

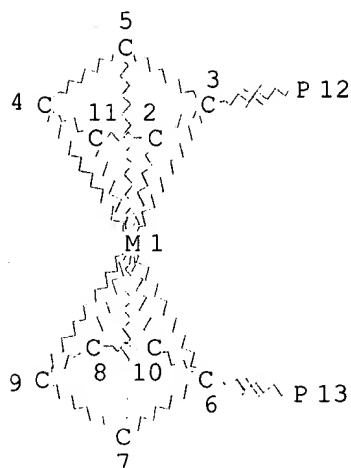
STEREO ATTRIBUTES: NONE

L9 SCR 2017

L11 7674 SEA FILE=REGISTRY SSS FUL L7 AND L9

L12 423 SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND (FE AND RH)/ELS

L13 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L15 3743 SEA FILE=REGISTRY SUB=L11 SSS FUL L13

L16 265 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L15

=> d his

(FILE 'HOME' ENTERED AT 07:07:27 ON 08 JAN 2004)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 07:07:47 ON 08 JAN 2004

L1 1 S (WO2000-GB3851 OR GB99-23952)/AP,PRN
E BURK M/AU
L2 127 S E3,E5,E11-E13
E GERLACH A/AU
L3 50 S E3,E4,E21
E CHIROTECH/PA,CS
L4 213 S E3-E31
SEL RN L1

FILE 'REGISTRY' ENTERED AT 07:10:11 ON 08 JAN 2004

L5 9 S E1-E9
E FERROCENE/CN
L6 1 S E3
L7 STR
L8 50 S L7
L9 SCR 2017
L10 50 S L7 AND L9
L11 7674 S L7 AND L9 FUL
SAV L11 LAVILLA700/A
L12 423 S L11 AND (FE AND RH)/ELS
L13 STR L7
L14 50 S L13 SAM SUB=L11
L15 3743 S L13 FUL SUB=L11
SAV L15 LAVILLA700A/A
L16 265 S L12 AND L15

L17 STR L13
L18 3 S L17 SAM SUB=L15
L19 142 S L17 FUL SUB=L15
SAV L19 LAVILLA700B/A
L20 26 S L16 AND L19
L21 20 S L20 AND 1/RH
L22 16 S L21 AND 2/P AND 1/FE
L23 4 S L21 NOT L22
L24 15 S L22 NOT C27H37F6FEO2P2RH

FILE 'HCAOLD' ENTERED AT 07:20:25 ON 08 JAN 2004

L25 0 S L24

FILE 'USPATFULL, USPAT2' ENTERED AT 07:20:29 ON 08 JAN 2004

L26 0 S L24

FILE 'HCAPLUS' ENTERED AT 07:20:33 ON 08 JAN 2004

L27 15 S L24
L28 5 S L27 AND L1-L4
E ALDEHYDE/CT
L29 386960 S E17+NT
L30 48009 S E3-E67
L31 502889 S ?ALDEHYD?
L32 1876 S L15
E HYDROGENATION/CT
L33 46596 S E3+NT
L34 36933 S E20+NT
L35 132 S E32+NT
L36 1397 S E36+NT
L37 104 S L16
L38 22 S L37 AND L29-L31
L39 7 S L38 AND L33-L36
L40 8 S L38 AND ?ALCOHOL?
L41 4 S L39 AND L40
L42 11 S L28,L39-L41
L43 1 S L27 AND P/DT
L44 21 S L27,L42,L43
L45 17 S L44 AND ?HYDROGENAT?
L46 9 S L45 AND L29-L31
L47 9 S L28,L46
L48 12 S L44,L45 NOT L47
SEL HIT RN L48

FILE 'REGISTRY' ENTERED AT 07:35:33 ON 08 JAN 2004

L49 13 S E1-E13
L50 10 S L49 AND L11

FILE 'HCAPLUS' ENTERED AT 07:36:42 ON 08 JAN 2004

L51 18 S L50
L52 15 S L51 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L53 4 S L47 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L54 19 S L28,L52,L53
L55 19 S L54 AND L1-L4,L27-L48,L51-L54
L56 4071 S PHOSPHOTUNGSTIC ACID
L57 2345 S PHOSPHOMOLYBDIC ACID
L58 1136 S SILICOTUNGSTIC ACID

FILE 'REGISTRY' ENTERED AT 07:39:46 ON 08 JAN 2004

L59 3 S 1343-93-7 OR 12026-57-2 OR 12027-38-2
L60 3 S 12534-77-9 OR 12379-13-4 OR 12363-31-4
L61 1638 S (12534-77-9 OR 12379-13-4 OR 12363-31-4)/CRN

FILE 'HCAPLUS' ENTERED AT 07:41:13 ON 08 JAN 2004

L62 3445 S L59 OR L60
L63 4365 S L61
L64 3 S L56-L58, L62-L63 AND L37
L65 2 S L16 AND ALUMINA

FILE 'REGISTRY' ENTERED AT 07:42:26 ON 08 JAN 2004

L66 1 S 1344-28-1

FILE 'HCAPLUS' ENTERED AT 07:42:40 ON 08 JAN 2004

L67 218225 S L66
L68 342015 S AL2O3 OR ALUMINUM OXIDE
L69 2 S L67, L68 AND L16
L70 0 S TETRAFLUOROETHYLENE PERFLUORO VINYL ETHER SULFONATE
L71 0 S TETRAFLUOROETHYLENE PERFLUORO VINYL ETHER SULPHONATE
L72 0 S TETRAFLUOROETHYLENE PERFLUOROVINYL ETHER SULPHONATE
L73 0 S TETRAFLUOROETHYLENE PERFLUOROVINYL ETHER SULFONATE
L74 0 S ?TETRAFLUOROETHYLENE? AND L16
L75 6 S ?VINYL? AND L16
L76 163 S ?TETRAFLUOROETHYLENE? (L) ?VINYL? (L) (?SULFONATE? OR ?SULPHON
L77 23774 S PTFE
L78 60 S L77 (L) ?VINYL? (L) (?SULFONATE? OR ?SULPHONATE?)

FILE 'REGISTRY' ENTERED AT 07:47:13 ON 08 JAN 2004

L79 1 S 9002-84-0
L80 1 S 116-14-3
L81 3998 S 116-14-3/CRN
L82 412 S L81 AND S/ELS
L83 76 S L82 AND NR>=1
L84 336 S L82 NOT L83
L85 247 S L84 NOT N/ELS
L86 97 S L85 AND 2/NC
L87 127 S L85 AND 3/NC
L88 23 S L85 NOT L86, L87
L89 244 S L85 NOT SI/ELS

FILE 'HCAPLUS' ENTERED AT 07:52:06 ON 08 JAN 2004

L90 0 S L89 AND L16
L91 0 S L79, L80 AND L16
L92 0 S L82 AND L16
L93 19 S L64, L65, L69, L55

FILE 'REGISTRY' ENTERED AT 07:53:24 ON 08 JAN 2004

FILE 'HCAPLUS' ENTERED AT 07:53:31 ON 08 JAN 2004

L94 19 S L93 AND (RH OR ?RHODIUM?)

FILE 'REGISTRY' ENTERED AT 07:55:34 ON 08 JAN 2004

FILE 'HCAPLUS' ENTERED AT 07:55:42 ON 08 JAN 2004
SEL HIT RN L94

FILE 'REGISTRY' ENTERED AT 07:57:38 ON 08 JAN 2004

L95 59 S E14-E72
L96 31 S L16 AND L95
L97 28 S L95 NOT L96
L98 12 S L97 AND L11
L99 16 S L97 NOT L98

FILE 'HCAPLUS' ENTERED AT 07:59:28 ON 08 JAN 2004

L100 26 S L96
L101 20 S L100 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
L102 16 S L101 AND L94
L103 4 S L101 NOT L102

L104 20 S L101-L103

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:01:16 ON 08 JAN 2004

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FILE COVERS 1907 - 8 Jan 2004 VOL 140 ISS 2

FILE LAST UPDATED: 6 Jan 2004 (20040106/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l104 all hitstr tot

L104 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:283853 HCAPLUS

DN 134:312797

ED Entered STN: 20 Apr 2001

TI Supported ferrocene-based catalysts for selective aldehyde hydrogenation

IN Burk, Mark Joseph; Gerlach, Arne

PA Chirotech Technology Limited, UK

SO PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM B01J031-22

ICS B01J031-28; C07C045-62

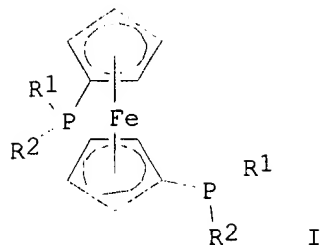
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 23, 67

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 2001026807	A1	20010419	WO 2000-GB3851	20001006 <--	
	W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
	RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
	EP 1222026	A1	20020717	EP 2000-964538	20001006 <--	
	R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL		
	JP 2003511229	T2	20030325	JP 2001-529860	20001006 <--	
PRAI	GB 1999-23952	A	19991008 <--			
	WO 2000-GB3851	W	20001006 <--			

OS MARPAT 134:312797
GI



- AB A supported catalyst comprises a cationic **rhodium** (I) complex of formula I, wherein R1 and R2 are the same or different C_≤30 hydrocarbyl groups, or R1 and R2 are linked to form a ring, and a heterogeneous support medium that provides anionic binding sites. Such a complex is particularly useful as a catalyst in a process of **hydrogenating an aldehyde** to produce the corresponding primary alc. Stirring 288 mg **phosphotungstic acid** with 4 g silica gel for 1 h, stirring the mixture with 64 mg [(DiPFc)Rh(COD)]BF₄ (COD = cyclooctadiene; DiPFc 1,1'-bis(diisopropylphosphino)ferrocene) gave a catalyst, which reduced pentanal to pentanol in 100% yield.
- ST supported ferrocene catalyst selective **aldehyde hydrogenation**; pentanal **hydrogenation** catalyst **rhodium** ferrocene complex
- IT Metallocenes
RL: CAT (Catalyst use); USES (Uses)
(ferrocenes; supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
- IT **Alcohols**, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(primary; supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
- IT **Hydrogenation catalysts**
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
- IT **Aldehydes, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
- IT 255064-36-9
RL: CAT (Catalyst use); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
- IT 7440-16-6DP, **Rhodium**, complex with 1,1'-bis(diisopropylphosphino)ferrocene, preparation 97239-80-0DP, 1,1'-Bis(diisopropylphosphino)ferrocene, **rhodium** complex.
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)
- IT 71-41-0P, n-Pentanol, preparation 505-10-2P 619-73-8P, p-Nitrobenzyl alcohol 636-72-6P, Thiophene-2-methanol 873-75-6P, p-Bromobenzyl alcohol 3446-90-0P, p-Methylthiobenzyl alcohol 6214-45-5P, p-Butoxybenzyl alcohol 79757-77-0P, 4-Bromo-Thiophene-2-methanol

RL: IMF (Industrial manufacture); PREP (Preparation)
(supported ferrocene-based catalysts for selective **aldehyde**
hydrogenation)

IT 98-03-3, 2-Formylthiophene 110-62-3, Pentanal
555-16-8, p-Nitrobenzaldehyde, reactions
1122-91-4, p-Bromobenzaldehyde 3268-49-3
3446-89-7, p-Thiomethylbenzaldehyde 5736-88-9, p-
Butoxybenzaldehyde 18791-75-8, 4-Bromo-2-Formylthiophene

RL: RCT (Reactant); RACT (Reactant or reagent)
(supported ferrocene-based catalysts for selective **aldehyde**
hydrogenation)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Burk, M; TETRAHEDRON LETTERS 1994, V35(28), P4963 HCAPLUS
- (2) Pugin, B; US 5783715 A 1998 HCAPLUS
- (3) Seton Hall University; WO 9828074 A 1998 HCAPLUS

IT 255064-36-9

RL: CAT (Catalyst use); USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde**
hydrogenation)

RN 255064-36-9 HCAPLUS

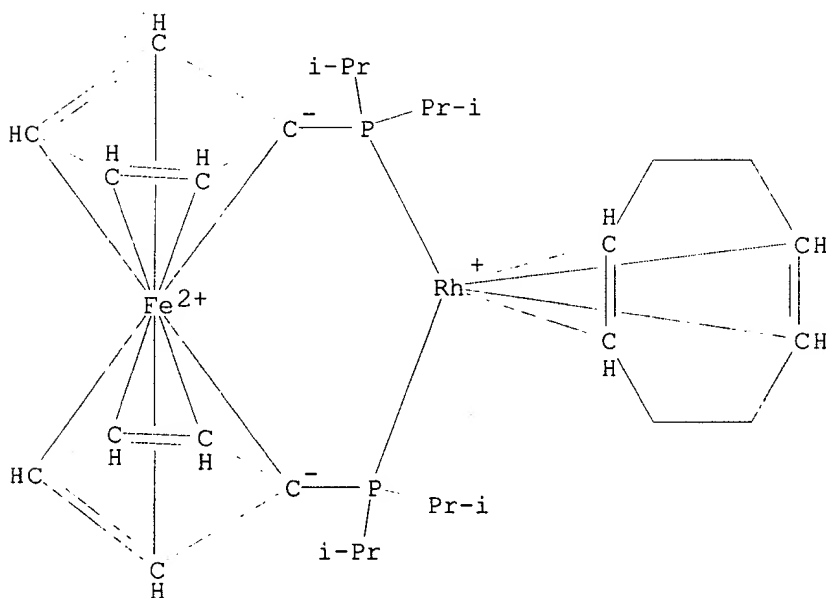
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-
κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-,
tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 157772-65-1

CMF C30 H48 Fe P2 Rh

CCI CCS

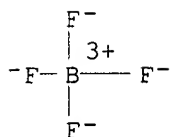


CM 2

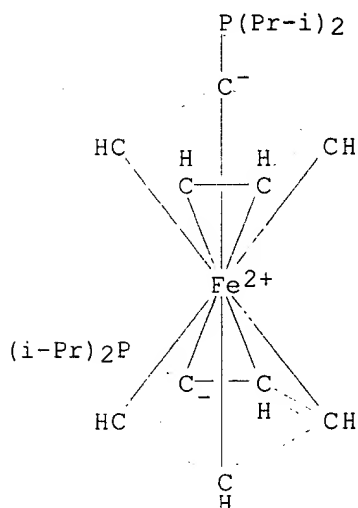
CRN 14874-70-5

CMF B F4

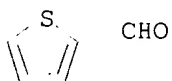
CCI CCS



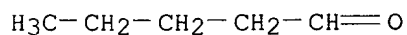
IT 97239-80-ODP, 1,1'-Bis(diisopropylphosphino)ferrocene,
rhodium complex
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
USES (Uses)
(supported ferrocene-based catalysts for selective **aldehyde**
hydrogenation)
RN 97239-80-0 HCAPLUS
CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



IT 98-03-3, 2-Formylthiophene 110-62-3, Pentanal
555-16-8, p-Nitrobenzaldehyde, reactions
1122-91-4, p-Bromobenzaldehyde 3268-49-3
3446-89-7, p-Thiomethylbenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(supported ferrocene-based catalysts for selective **aldehyde**
hydrogenation)
RN 98-03-3 HCAPLUS
CN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



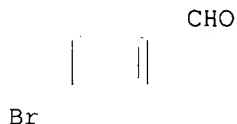
RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)



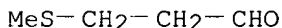
RN 555-16-8 HCAPLUS
CN Benzaldehyde, 4-nitro- (9CI) (CA INDEX NAME)



RN 1122-91-4 HCAPLUS
 CN Benzaldehyde, 4-bromo- (9CI) (CA INDEX NAME)



RN 3268-49-3 HCAPLUS
 CN Propanal, 3-(methylthio)- (9CI) (CA INDEX NAME)



RN 3446-89-7 HCAPLUS
 CN Benzaldehyde, 4-(methylthio)- (9CI) (CA INDEX NAME)



L104 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1999:767776 HCAPLUS
 DN 132:108089
 ED Entered STN: 06 Dec 1999
 TI Phosphines versus phosphinites as ligands in the **rhodium**
 catalyzed asymmetric **hydrogenation** of imines: a systematic study
 AU Tararov, Vitali I.; Kadyrov, Renat; Riermeier, Thomas H.; Holz, Jens;
 Borner, Armin
 CS Institut für Organische Katalyseforschung an der Universität Rostock e.V.,
 Rostock, D-18055, Germany
 SO Tetrahedron: Asymmetry (1999), 10(20), 4009-4015
 CODEN: TASYE3; ISSN: 0957-4166
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 67
 OS CASREACT 132:108089
 AB The asym. **hydrogenation** of N-(1-phenylethylidene)benzylamine
 with a range of **Rh**(I)-diphosphine and diphosphinite catalysts
 was studied. The reaction is strongly sensitive to the size of the metal
 chelate. Complexes based on five- and six-membered chelates or
 electron-rich alkylphosphines gave poor or moderate conversions. The
 reactivity of diphosphine catalysts could be increased by the addition of
 p-toluenesulfonic acid. Unexpectedly, **Rh**-complexes based on
 chiral diphosphinites and a diphosphite also rapidly converted the
 substrate to the desired amine. Highest efficiency was observed with a

Rh(I) complex with (R,R)-1,2-cyclohexanol-bisdiphenylphosphinite [(R,R)-bdpchi] as chiral ligand. Without any additive complete **hydrogenation** of the imine was achieved within 5 h. The product was produced in an enantioselectivity of 71%.

ST phosphine phosphinite ligand comparison **rhodium** catalyzed asym **hydrogenation** imine

IT Phosphines

RL: CAT (Catalyst use); USES (Uses)

(diphosphines; phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT Amines, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

IT Imines

RL: RCT (Reactant); RACT (Reactant or reagent)

(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT **Hydrogenation**

Hydrogenation catalysts

(stereoselective; phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT 14428-98-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(: (phosphine)- and (phosphinite)**rhodium**-catalyzed asym. **hydrogenation** of)

IT 53450-79-6 60104-68-9 60430-43-5 63569-12-0 66787-44-8
72611-80-4 79255-71-3 82796-32-5 109143-86-4 163161-28-2
171561-30-1 171561-32-3 180420-80-8 185754-11-4 187886-92-6
204762-36-7 214827-80-2 217818-18-3 237058-40-1 255064-34-7
255064-35-8 255064-36-9 255064-38-1 255064-68-7
255719-90-5

RL: CAT (Catalyst use); USES (Uses)

(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

IT 17480-69-2P 38235-77-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Achiwa, K; J Am Chem Soc 1976, V98, P8265 HCAPLUS
- (2) Bakos, J; J Chem Soc, Chem Commun 1991, P1684 HCAPLUS
- (3) Bomer, A; Tetrahedron Lett 1994, V35, P6071
- (4) Borns, S; Eur J Inorg Chem 1998, P1291 HCAPLUS
- (5) Borns, S; Tetrahedron: Asymmetry 1999, V10, P1425 HCAPLUS
- (6) Broger, E; Tetrahedron: Asymmetry 1998, V9, P4043 HCAPLUS
- (7) Burk, M; J Am Chem Soc 1992, V114, P6266 HCAPLUS
- (8) Cahill, J; Tetrahedron: Asymmetry 1998, V9, P4307 HCAPLUS
- (9) Cullen, W; J Mol Catal 1990, V62, P243 HCAPLUS
- (10) Cullen, W; J Mol Catal 1990, V62, P243 HCAPLUS
- (11) Holz, J; Tetrahedron: Asymmetry 1995, V6, P1973 HCAPLUS
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- (15) Kobayashi, S; Chem Rev 1999, V99, P1069 HCAPLUS
- (16) Krause, H; J Mol Catal A: Chemical 1995, V104, P147 HCAPLUS
- (17) Krause, H; New J Chem 1989, V13, P615 HCAPLUS
- (18) Kumar, A; Angew Chem 1994, V106, P2272 HCAPLUS
- (19) Kumar, A; Angew Chem, Int Ed Engl 1994, V33, P2197
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- (22) Ng Cheon Chan, Y; J Am Chem Soc 1990, V112, P940
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 (24) Ojima, I; Catalytic Asymmetric Synthesis 1993, P31
 (25) Ringwald, M; J Am Chem Soc 1999, V121, P1524 HCAPLUS
 (26) Sablong, R; Tetrahedron Lett 1997, V37, P4937
 (27) Sablong, R; Tetrahedron: Asymmetry 1996, V7, P3059 HCAPLUS
 (28) Schnider, P; Chem Eur J 1997, V3, P887 HCAPLUS
 (29) Selke, R; J Mol Catal 1986, V37, P213 HCAPLUS
 (30) Selke, R; Tetrahedron 1996, V52, P15079 HCAPLUS
 (31) Spindler, F; Angew Chem 1990, V102, P561 HCAPLUS
 (32) Spindler, F; Angew Chem, Int Ed Engl 1990, V29, P558
 (33) Spindler, F; Transition Metals for Organic Synthesis 1998, V2, P69 HCAPLUS
 (34) Tanaka, M; J Chem Soc, Chem Commun 1975, P735 HCAPLUS
 (35) Tani, K; Chem Lett 1995, P955 HCAPLUS
 (36) Tani, K; Chem Lett 1995, P955 HCAPLUS
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IT 255064-35-8 255064-36-9

RL: CAT (Catalyst use); USES (Uses)

(phosphines vs. phosphinites as ligands in the rhodium
 catalyzed asym. hydrogenation of imines)

RN 255064-35-8 HCAPLUS

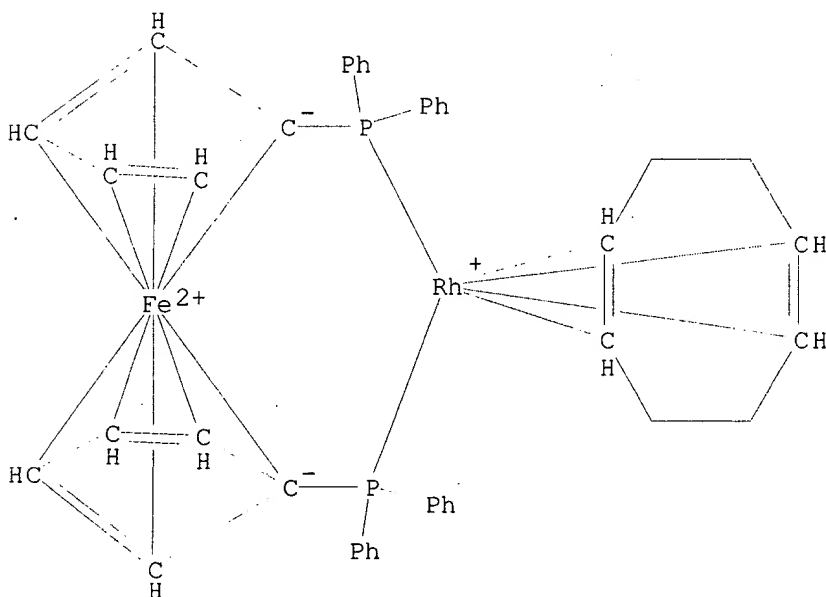
CN Rhodium(1+), [1,1'-bis(diphenylphosphino-κP)ferrocene][(1,2,5,6-
 η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 91159-09-0

CMF C42 H40 Fe P2 Rh

CCI CCS

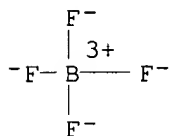


CM 2

CRN 14874-70-5

CMF B F4

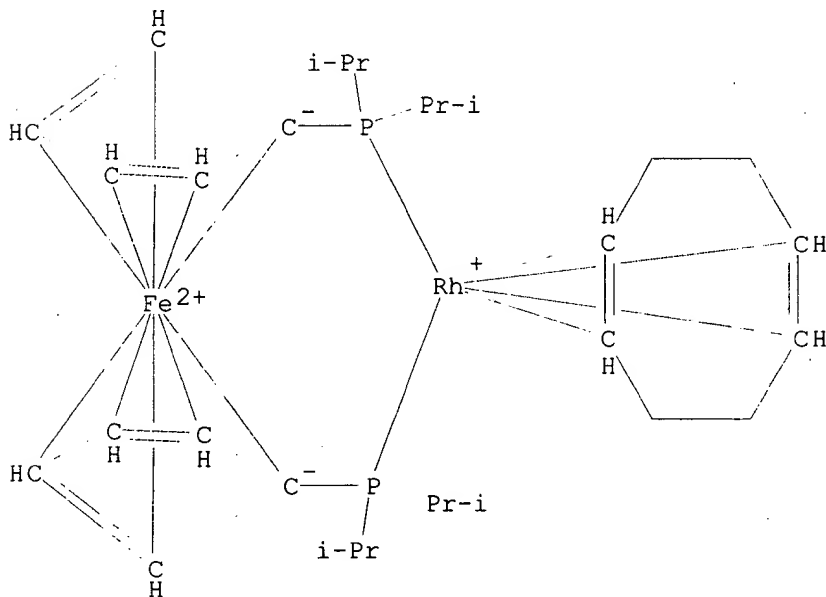
CCI CCS



RN 255064-36-9 HCAPLUS
 CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-
 κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-,
 tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

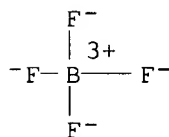
CM 1

CRN 157772-65-1
 CMF C30 H48 Fe P2 Rh
 CCI CCS



CM 2

CRN 14874-70-5
 CMF B F4
 CCI CCS



DN 129:303986
 ED Entered STN: 22 Oct 1998
 TI Processes and catalysts for producing **hydroxyaldehydes**
 IN Briggs, John Robert; Packett, Diane Lee; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Olson, Kurt Damar; Tjaden, Erik Bruce; Guram, Anil Sakharam; Eisenschmid, Thomas Carl; Brigham, Elaine Susan
 PA Union Carbide Chemicals & Technology Corp., USA
 SO U.S., 36 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07C045-50
 NCL 568454000
 CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5821389	A	19981013	US 1997-843339	19970415 <--
	CN 1222903	A	19990714	CN 1997-195721	19970423 <--
PRAI	US 1997-843339		19970415	<--	

OS MARPAT 129:303986

AB This invention relates in part to processes for producing one or more substituted or unsubstituted **hydroxyaldehydes**, e.g., 6-hydroxyhexanals, which comprise subjecting one or more substituted or unsubstituted alkadienes, e.g., butadiene, to reductive hydroformylation in the presence of a reductive hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and hydroformylation in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, to produce one or more substituted or unsubstituted **hydroxyaldehydes**. The substituted and unsubstituted **hydroxyaldehydes** produced by the processes of this invention can undergo further reaction(s) to afford desired derivs. thereof, e.g., epsilon caprolactone. This invention also relates in part to reaction mixts. containing one or more substituted or unsubstituted **hydroxyaldehydes** as principal product(s) of reaction.

ST **hydroxyaldehyde** manuf diene hydroformylation; metal organophosphorus ligand complex catalyst hydroformylation

IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (**hydroxy**; processes and catalysts for producing **hydroxyaldehydes**)

IT Hydroformylation
 Hydroformylation catalysts
 (processes and catalysts for producing **hydroxyaldehydes**)

IT Alkadienes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (processes and catalysts for producing **hydroxyaldehydes**)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 607-01-2, Ethyldiphenylphosphine 998-40-3, Tributylphosphine 1605-53-4, Diethylphenylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4706-17-6 4731-53-7, Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4 **12150-46-8** 14874-82-9, **Rhodium** dicarbonyl acetylacetonate 17005-57-1 19262-01-2, Cyclohexyldiethylphosphine 32305-98-9 32376-20-8, t-Butyldiethylphosphine 50420-43-4, n-Butyldiethylphosphine 53111-20-9, Diphenyl(o-methoxyphenyl)phosphine 76189-55-4, (R)-(+)-2,2'-Bis(diphenylphosphino)-1,1'-binaphthyl **84680-96-6** 108793-33-5 111982-81-1, 2,2'-(Bisdiphenylphosphinomethyl)1,1'-biphenyl 121627-17-6 138776-88-2 138776-89-3 154813-98-6 154814-02-5 169254-16-4 198475-94-4 198478-30-7 198478-33-0
 RL: CAT (Catalyst use); USES (Uses)
 (processes and catalysts for producing **hydroxyaldehydes**)

IT 34067-76-0P, 6-Hydroxyhexanal
RL: IMF (Industrial manufacture); PREP (Preparation)
(processes and catalysts for producing **hydroxyaldehydes**)

IT 764-37-4P, trans-3-Penten-1-ol 764-38-5P, cis-3-Penten-1-ol 821-09-0P,
4-Penten-1-ol 1576-95-0P, cis-2-Penten-1-ol 1576-96-1P,
trans-2-Penten-1-ol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)
(processes and catalysts for producing **hydroxyaldehydes**)

IT 106-99-0, Butadiene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(processes and catalysts for producing **hydroxyaldehydes**)

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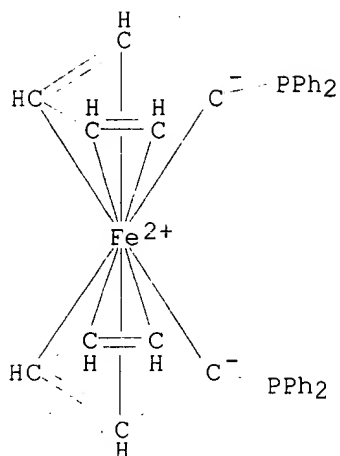
RE

(1) Anderson, J; Chem Commun 1996, P1543
(2) Anon; GB 1254222 1971 HCAPLUS
(3) Anon; GB 1357735 1974 HCAPLUS
(4) Anon; EP 0183545 1985 HCAPLUS
(5) Anon; EP 0343819 1989 HCAPLUS
(6) Anon; EP 0420510 1991 HCAPLUS
(7) Anon; EP 0448848 1991 HCAPLUS
(8) Bahrmann; US 5583250 1996 HCAPLUS
(9) Billig; US 4769498 1986 HCAPLUS
(10) Carlock; US 4185038 1980 HCAPLUS
(11) Carlock; US 4189448 1980 HCAPLUS
(12) Carlock; US 4214109 1980 HCAPLUS
(13) Dennis; US 4482749 1984 HCAPLUS
(14) Dennis; US 4567306 1996 HCAPLUS
(15) Fell; US 5434312 1995 HCAPLUS
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(19) Hoshiyama; US 4447661 1984 HCAPLUS
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(21) Johnson; US 4409418 1983 HCAPLUS
(22) Kim; US 4198352 1980 HCAPLUS
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(30) Oswald; US 4528404 1985 HCAPLUS
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P186
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(36) Smith; US 4224255 1980 HCAPLUS
(37) van Vliet; US 4647707 1987 HCAPLUS
(38) Vargas; US 5306848 1994 HCAPLUS
(39) Yates; US 4443638 1984 HCAPLUS
(40) Young; US 4625068 1986 HCAPLUS

IT 12150-46-8 84680-96-6
RL: CAT (Catalyst use); USES (Uses)
(processes and catalysts for producing **hydroxyaldehydes**)

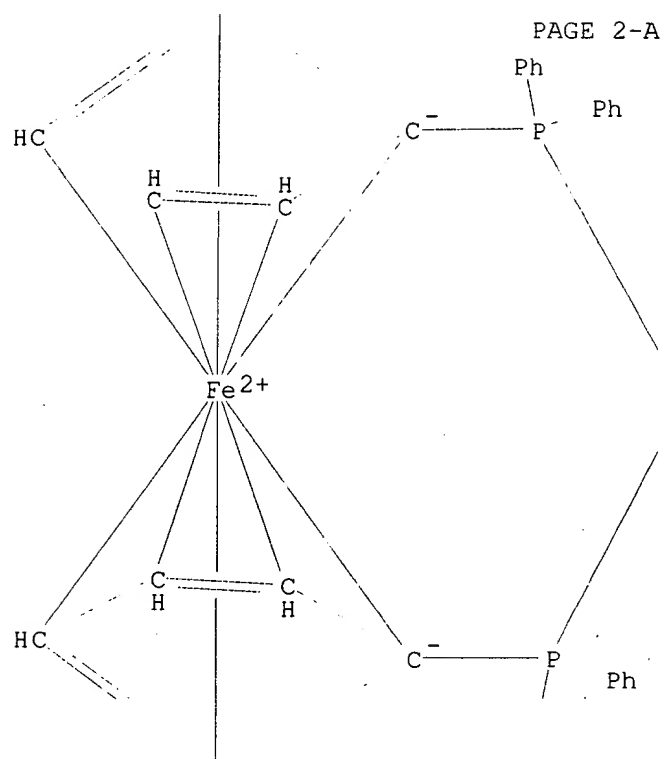
RN 12150-46-8 HCAPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)

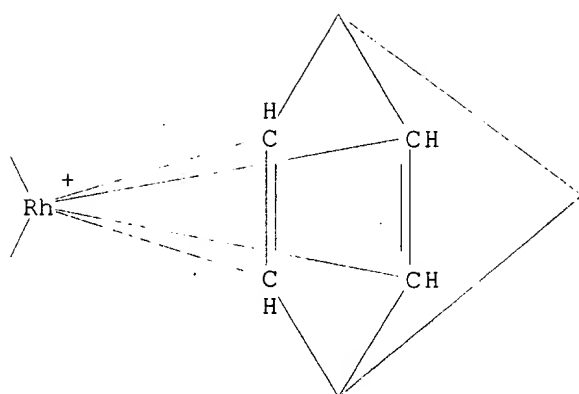


RN 84680-96-6 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)
 CM 1
 CRN 79790-97-9
 CMF C41 H36 Fe P2 Rh
 CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A

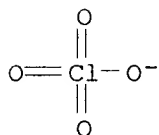
Ph

C
H

CM 2

CRN 14797-73-0

CMF C1 04



L104 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:756953 HCAPLUS

DN 128:14354

ED Entered STN: 04 Dec 1997

TI Selective manufacture of alkenals and alkenols by hydroformylation of
alkadienes and catalysts thereforIN Packett, Diane Lee; Briggs, John Robert; Bryant, David Robert; Phillips,
Ailene Gardner

PA Union Carbide Chemicals and Plastics Technology Corp., USA

SO PCT Int. Appl., 109 pp.

CODEN: PIXXD2

DT Patent

LA English

IC C07C045-49; C07C047-21; C07C029-141; C07C033-025

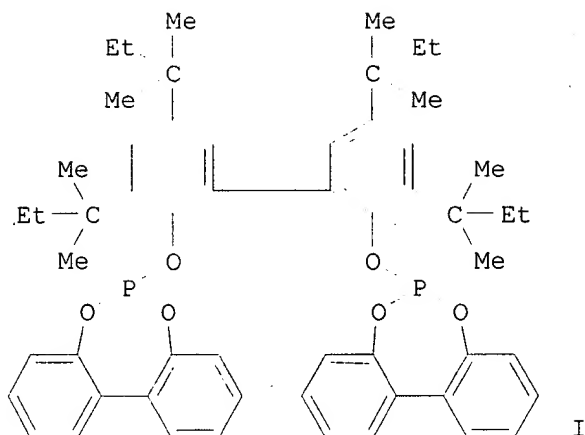
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 67

FAN.CNT 7

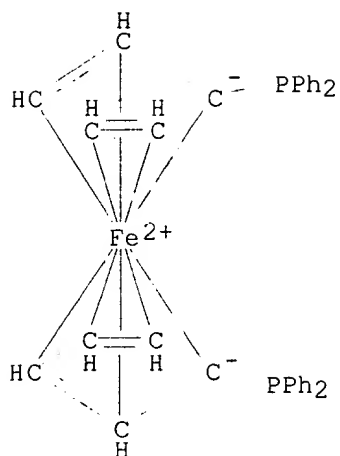
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	RW:	GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
	US 5886237	A	19990323	US 1997-843389	19970415 <--
	US 6187970	B1	20010213	US 1997-843390	19970415 <--
	AU 9727422	A1	19971112	AU 1997-27422	19970423 <--
	EP 853609	A1	19980722	EP 1997-921365	19970423 <--
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PRAI	US 1996-15944P	P	19960424	<--	
	US 1996-15953P	P	19960424	<--	
	US 1996-16116P	P	19960424	<--	
	US 1996-16287P	P	19960424	<--	
	US 1997-843389	A	19970415	<--	

US 1997-842665 A 19970415 <--
 WO 1997-US6889 W 19970423 <--
 OS MARPAT 128:14354
 GI



- AB Substituted or unsubstituted alkadienes, e.g., butadiene, or a mixture thereof are hydroformylated in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and at an alkadiene and/or carbon monoxide partial pressure sufficient to selectively produce ≥ 1 (un)substituted alkenal, e.g., pentenal. The (un)substituted alkenals can undergo further reaction(s) to afford desired derivs., e.g., **hydrogenation** to alkenols, particularly pentenols. The invention also relates to reaction mixts. containing ≥ 1 (un)substituted alkenals or alkenols as principal product(s) of the reactions. Thus, liquid butadiene was charged to a reactor containing a THF solution of **rhodium** dicarbonylacetylacetonate (200 ppm Rh) and 6,6'-[[3,3',5,5'-tetrakis(1,1-dimethylpropyl)-[1,1'-biphenyl]-1,1'-diyl]bis(oxy)]bis-dibenzo[d,f][1,3,2]dioxaphosphepin (I) (12:1 ligand-Rh ratio), heated to 95° and pressurized to 500 psig with 1:1 CO-H₂ to give, after 2 h, 95% butadiene conversion to 3-pentenals 75, 4-pentenal 3, 2-pentenals 5, **valeraldehyde** 7, branched **dialdehyde** 1, and **adipaldehyde** 9%.
- ST alkadiene hydroformylation alkenal alkenol manuf; butadiene hydroformylation alkenal alkenol catalyst; **rhodium** phosphine ligand hydroformylation catalyst; pentenal manuf hydroformylation butadiene
- IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (C5; selective manufacture of **alkenals** and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (alkenals; selective manufacture of **alkenals** and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT **Alcohols, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (alkenols; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT **Dialdehydes**
 RL: BYP (Byproduct); PREP (Preparation)

- (formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT Hydroformylation catalysts
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 1038-95-5, Tris(p-tolyl)phosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 6372-40-3, Isopropylidiphenylphosphine 6737-42-4 **12150-46-8** 14874-82-9, Rhodium dicarbonyl acetylacetonate 32305-98-9 53111-20-9 61806-56-2, Phenylbis(cyanomethyl)phosphine **84680-96-6** 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6 198475-94-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT **110-62-3P, Valeraldehyde** 629-11-8P, 1,6-Hexanediol 1072-21-5P, **Adipaldehyde** 34067-76-0P, 6-Hydroxyhexanal
RL: BYP (Byproduct); PREP (Preparation)
(formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT **96-17-3P, 2-Methylbutyraldehyde** 25167-67-3P, Butene 100080-07-7P
RL: BYP (Byproduct); PREP (Preparation)
(formation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT 106-99-0, Butadiene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT 764-37-4DP, trans-3-Penten-1-ol, derivs. 764-37-4P, trans-3-Penten-1-ol 764-38-5DP, cis-3-Penten-1-ol, derivs. 764-38-5P, cis-3-Penten-1-ol 821-09-0DP, 4-Penten-1-ol, derivs. 821-09-0P, 4-Penten-1-ol 1576-86-9DP, cis-2-Pentenal, derivs. 1576-86-9P, cis-2-Pentenal 1576-87-0DP, trans-2-Pentenal, derivs. 1576-87-0P, trans-2-Pentenal 1576-95-0DP, cis-2-Penten-1-ol, derivs. 1576-95-0P, cis-2-Penten-1-ol 1576-96-1DP, trans-2-Penten-1-ol, derivs. 1576-96-1P, trans-2-Penten-1-ol 2100-17-6DP, 4-Pentenal, derivs. 2100-17-6P, 4-Pentenal 53448-06-9DP, cis-3-Pentenal, derivs. 53448-06-9P 58838-14-5DP, derivs. 58838-14-5P, trans-3-Pentenal
RL: IMF (Industrial manufacture); PREP (Preparation)
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT 106-99-0D, Butadiene, derivs. 630-08-0, Carbon monoxide, reactions 1333-74-0, Hydrogen, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- IT **12150-46-8 84680-96-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)
- RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)

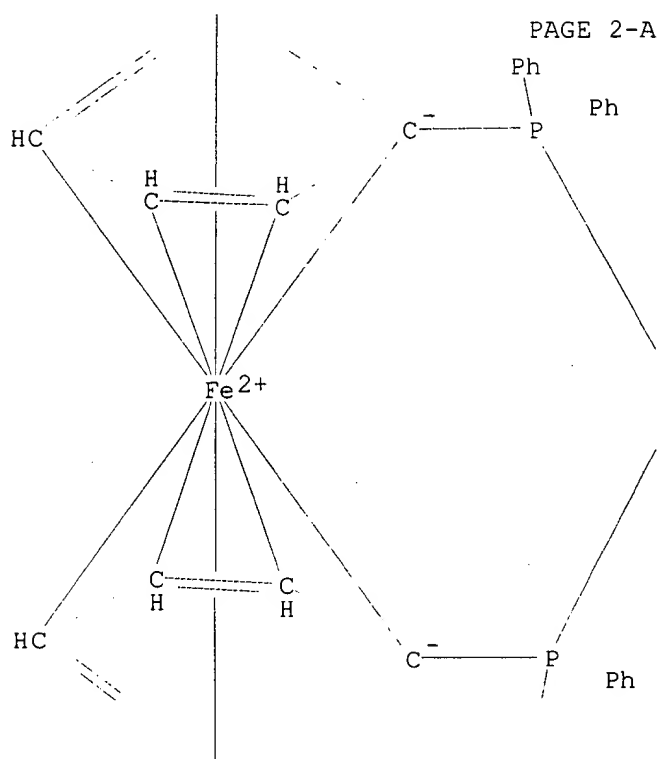


RN 84680-96-6 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

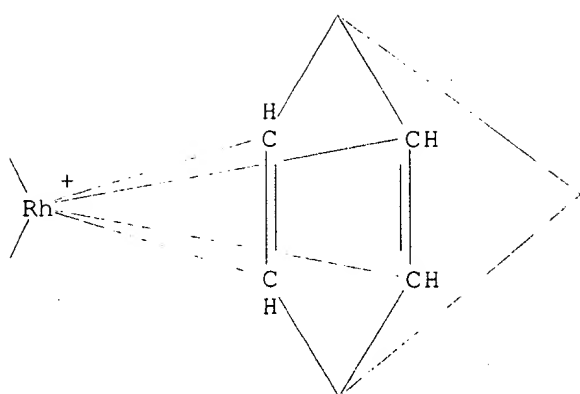
CM 1

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A

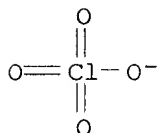
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CM 2

CRN 14797-73-0

CMF Cl O4



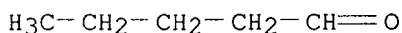
IT 110-62-3P, Valeraldehyde

RL: BYP (Byproduct); PREP (Preparation)

(formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

RN 110-62-3 HCAPLUS

CN Pentanal (9CI) (CA INDEX NAME)



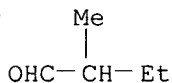
IT 96-17-3P, 2-Methylbutyraldehyde

RL: BYP (Byproduct); PREP (Preparation)

(formation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

RN 96-17-3 HCAPLUS

CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)



L104 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:756952 HCAPLUS

DN 128:14353

ED Entered STN: 04 Dec 1997

TI Manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor

IN Briggs, John Robert; Packett, Diane Lee; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Olson, Kurt Damar; Tjaden, Erick Bruce; Guram, Anil Sakharam; Eisenschmid, Thomas Carl; Bragham, Elaine Susan

PA Union Carbide Chemicals and Plastics Technology Corp., USA

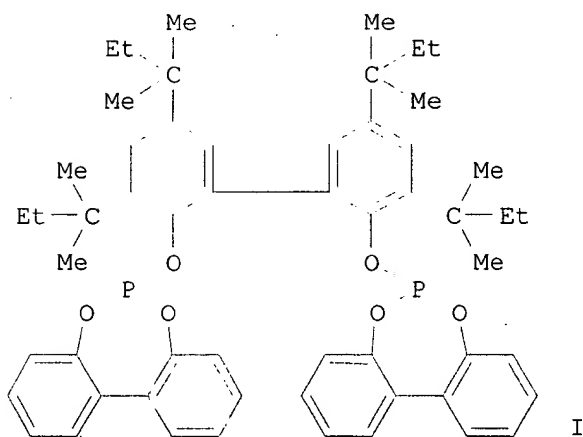
SO PCT Int. Appl., 113 pp.

CODEN: PIXXD2

DT Patent
 LA English
 IC C07C045-49; C07C043-68; C07C029-16; C07C045-50; C07C047-19
 CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 Section cross-reference(s): 35, 67

FAN.CNT 6

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PI	WO 9740001	A1	19971030	WO 1997-US6881	19970423 <--
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	RW:	GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
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	EP 900187	A1	19990310	EP 1997-921364	19970423 <--
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	AT 223368	E	20020915	AT 1997-921364	19970423 <--
	ES 2178775	T3	20030101	ES 1997-921364	19970423 <--
	ES 2185006	T3	20030416	ES 1997-918801	19970423 <--
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	US 1996-16259P	P	19960424 <--		
	US 1996-16263P	P	19960424 <--		
	US 1996-16378P	P	19960424 <--		
	US 1997-843340	A	19970415 <--		
	WO 1997-US6881	W	19970423 <--		
OS	MARPAT 128:14353				
GI					



AB Substituted or unsubstituted **hydroxyaldehydes**, e.g., 6-hydroxyhexanals, are prepared by reductive hydroformylation of ≥ 1 (un)substituted alkadienes, e.g., butadiene, or pentenals in the presence of a reductive hydroformylation catalyst; e.g., a metal-organophosphorus

ligand complex catalyst, and hydroformylation of the unsatd. **alcs** in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst. The (un)substituted **hydroxyaldehydes** can undergo further reaction(s) to afford desired derivs., e.g., ϵ -caprolactone (no data). Thus, liquid butadiene was charged to a reactor containing a THF solution of **rhodium** dicarbonyl acetylacetonate (200 ppm Rh) and 6,6'-[[3,3',5,5'-tetrakis(1,1-dimethylpropyl)[1,1'-biphenyl]-2,2'-diyl]bis(oxy)]bis-dibenzo[d,f][1,3,2]dioxaphosphin (I) (12:1 ligand-Rh ratio), heated to 95° and pressurized to 500 psig with 1:1 CO-H₂, giving, after 2 h, 95% butadiene conversion to 3-pentenals 75, 4-pentenal 3, 2-pentenals 5, **valeraldehyde** 7, branched **dialdehyde** 1, and **adipaldehyde** 9%.

- ST **hydroxyaldehyde** manuf hydroformylation alkadiene pentenal
alc; metal organophosphorus ligand hydroformylation catalyst;
 butadiene reductive hydroformylation catalyst **hydroxyaldehyde**
 manuf; **rhodium** dicarbonyl acetylacetonate hydroformylation
 catalyst; phosphine ligand hydroformylation catalyst
- IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (C5, preparation of; in manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd.
alcs. and catalysts therefor)
- IT **Dialdehydes**
 RL: BYP (Byproduct); PREP (Preparation)
 (branched, formation of; in manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd. **alcs.**
 and catalysts therefor)
- IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (**hydroxy**; manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd.
alcs. and catalysts therefor)
- IT Hydroformylation catalysts
 (manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)
- IT Alkadienes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)
- IT **Alcohols, reactions**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (unsatd.; manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)
- IT 96-17-3P, 2-Methylbutyraldehyde 110-62-3P,
Valeraldehyde 764-39-6P, 2-Pentenal 1072-21-5P,
Adipaldehyde 2100-17-6P, 4-Pentenal 5604-55-7P, 3-Pentenal
 25167-67-3P, Butene 100080-07-7P
 RL: BYP (Byproduct); PREP (Preparation)
 (byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes or pentenals and catalysts therefor)
- IT 71-41-ODP, Pentan-1-ol, derivs. 110-62-3DP,
Valeraldehyde, derivs. 111-30-8DP, 1,5-Pentanediol,
 derivs. 638-37-9DP, 1,4-Butanediol, derivs. 1072-21-5DP,
 1,6-Hexanediol, derivs.
 RL: BYP (Byproduct); PREP (Preparation)
 (byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)
- IT 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses

607-01-2, Ethyldiphenylphosphine 672-66-2 1038-95-5,
 Tris(p-tolyl)phosphine 1605-53-4, Diethylphenylphosphine 2234-97-1,
 Tripropylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4731-53-7,
 Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4
12150-46-8 14874-82-9, **Rhodium** dicarbonyl
 acetylacetonate 19262-01-2 32305-98-9 32376-20-8,
 tert-Butyldiethylphosphine 50420-43-4 53111-20-9 **84680-96-6**
 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6
 198475-94-4

RL: CAT (Catalyst use); USES (Uses)

(catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes or pentenals and catalysts therefor)

IT 19584-30-6, **Tetrarhodium** dodecacarbonyl 76189-55-4
 111982-81-1, 2,2'-(Bisdiphenylphosphinomethyl)-1,1'-biphenyl 154814-02-5
 169254-16-4 198478-30-7 198478-33-0 198478-35-2

RL: CAT (Catalyst use); USES (Uses)

(catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of
 unsatd. **alcs.** and catalysts therefor)

IT 764-37-4P, trans-3-Penten-1-ol 60544-74-3P, 2-Pentenol

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)

(formation and reaction of; manufacture of **hydroxyaldehydes** by
 hydroformylation of unsatd. **alcs.** and catalysts therefor)

IT 71-41-0P, 1-Pentanol, preparation

RL: BYP (Byproduct); PREP (Preparation)

(formation in hydroformylation of cis-3-pentenol; manufacture of
hydroxyaldehydes by hydroformylation of unsatd. **alcs.**
 and catalysts therefor)

IT 106-99-0D, Butadiene, derivs.

RL: RCT (Reactant); RACT (Reactant or reagent)

(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes
 and catalysts therefor)

IT 106-99-0, Butadiene, reactions 630-08-0, Carbon monoxide, reactions
 1333-74-0, Hydrogen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes
 or pentenals and catalysts therefor)

IT 4221-03-8DP, 5-Hydroxypentanal, derivs. 4221-03-8P, 5-Hydroxypentanal
 25714-71-0DP, 4-Hydroxybutanal, derivs. 25714-71-0P, 4-Hydroxybutanal
 34067-76-0DP, 6-Hydroxyhexanal, derivs. 34067-76-0P, 6-Hydroxyhexanal

RL: IMF (Industrial manufacture); PREP (Preparation)

(manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)

IT 31424-04-1D, Pentenal, derivs.

RL: RCT (Reactant); RACT (Reactant or reagent)

(manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)

IT 764-38-5, cis-3-Pentenol

RL: RCT (Reactant); RACT (Reactant or reagent)

(manufacture of **hydroxyaldehydes** by hydroformylation of unsatd.
alcs. and catalysts therefor)

IT 156619-80-6P, Penten-1-ol

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and reaction of; manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd. **alcs.**
 and catalysts therefor)

IT 156619-80-6D, Penten-1-ol, derivs.

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and reaction of; manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd. **alcs.**

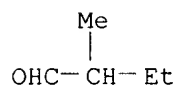
and catalysts therefor)

IT 821-09-0P, 4-Pentenol 1576-95-0P, cis-2-Penten-1-ol 1576-96-1P, trans-2-Penten-1-ol
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs.** and catalysts therefor)

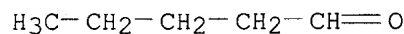
IT 695-06-7P 18545-19-2P
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (preparation of; manufacture of **hydroxyaldehydes** by hydroformylation of unsatd. **alcs.** and catalysts therefor)

IT 96-17-3P, 2-Methylbutyraldehyde 110-62-3P, Valeraldehyde
 RL: BYP (Byproduct); PREP (Preparation)
 (byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

RN 96-17-3 HCAPLUS
 CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)

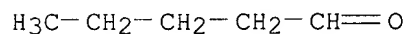


RN 110-62-3 HCAPLUS
 CN Pentanal (9CI) (CA INDEX NAME)

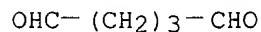


IT 110-62-3DP, Valeraldehyde, derivs. 111-30-8DP, 1,5-Pentanediol, derivs.
 RL: BYP (Byproduct); PREP (Preparation)
 (byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

RN 110-62-3 HCAPLUS
 CN Pentanal (9CI) (CA INDEX NAME)

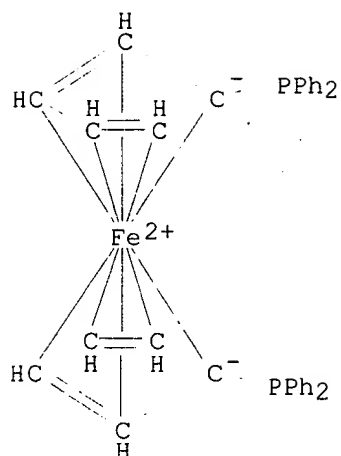


RN 111-30-8 HCAPLUS
 CN Pentanediol (9CI) (CA INDEX NAME)



IT 12150-46-8 84680-96-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

RN 12150-46-8 HCAPLUS
 CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)

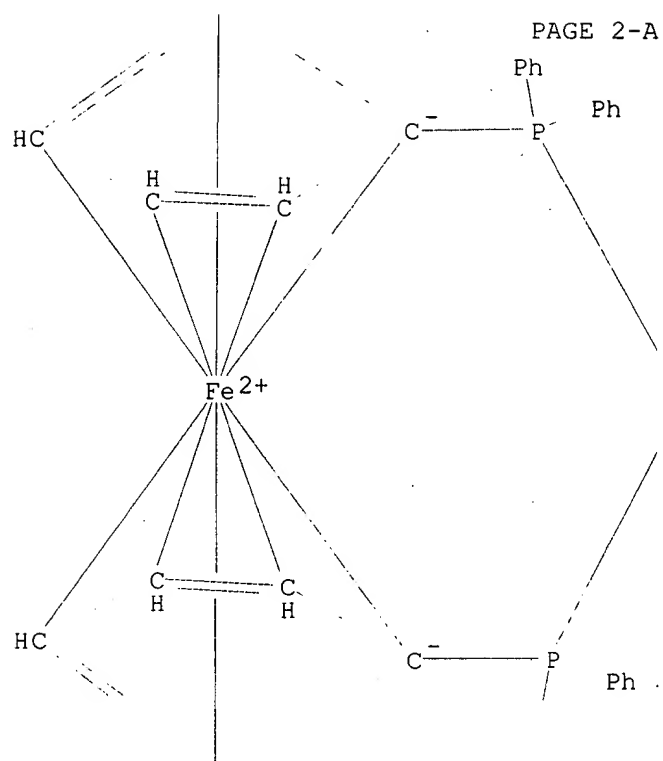


RN 84680-96-6 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

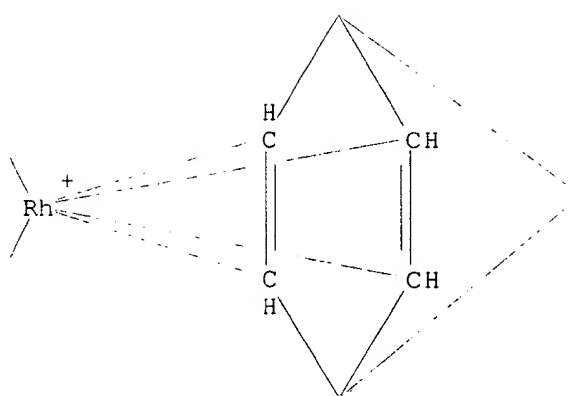
CM 1

CRN 79790-97-9
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 CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A

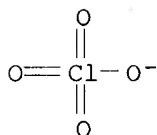
Ph

C
H

CM 2

CRN 14797-73-0

CMF C1 O4



L104 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:740058 HCAPLUS

DN 128:13065

ED Entered STN: 24 Nov 1997

TI Preparation of alkenols by reductive hydroformylation of alkadienes.

IN Packett, Diane Lee; Briggs, John Robert; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Guram, Anil Sakham; Olson, Kurt Dawar; Eisenschmid, Thomas Carl; Tjaden, Erik Bruce

PA Union Carbide Chemicals and Plastics Technology Corp., USA

SO PCT Int. Appl., 103 pp.

CODEN: PIXXD2

DT Patent

LA English

IC C07C029-16; C07C031-20

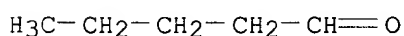
CC 23-7 (Aliphatic Compounds)

FAN.CNT 7

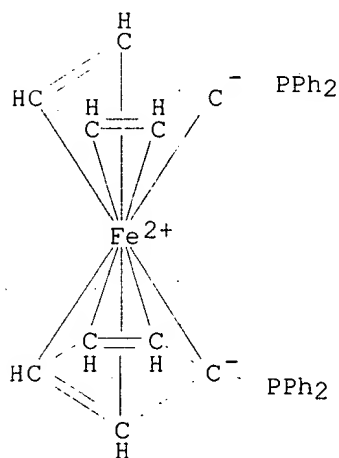
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PI	WO 9739996	A1	19971030	WO 1997-US6852	19970423 <--
	W:	AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
	US 6187970	B1	20010213	US 1997-843390	19970415 <--
	US 2002007096	A1	20020117	US 1997-842666	19970415 <--
	AU 9728093	A1	19971112	AU 1997-28093	19970423 <--
	US 6369283	B1	20020409	US 2000-704411	20001102 <--
PRAI	US 1996-15947P	P	19960424 <--		
	US 1996-16287P	P	19960424 <--		
	US 1997-842666	A	19970415 <--		
	US 1997-843381	A3	19970415 <--		
	WO 1997-US6852	W	19970423 <--		
OS	CASREACT 128:13065; MARPAT 128:13065				
AB	Catalytic reductive hydroformylation of ≥ 1 alkadiene selectively produces ≥ 1 (substituted) alkenol. Thus, a solution of				

rhodium dicarbonyl acetylacetonate and trioctylphosphine in octanol was pressurized with butadiene and 600 psi CO/200 psi H₂ and heated at 80° to give 98% butadiene conversion and 88% selectivity for 3- and 4-pentenols.

- ST butadiene reductive hydroformylation; alkenol prepn; pentenol prepn;
alkadiene reductive hydroformylation
- IT **Alcohols**, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(alkenols; preparation of alkenols by reductive hydroformylation of alkadienes)
- IT Hydroformylation catalysts
(**dicarbonylacetylacetonatorhodium**(I) with phosphine ligands for reductive hydroformylation; preparation of alkenols by reductive hydroformylation of alkadienes)
- IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of alkenols by reductive hydroformylation of alkadienes)
- IT Hydroformylation
(reductive hydroformylation; preparation of alkenols by reductive hydroformylation of alkadienes)
- IT 71-41-0P, 1-Pentanol, preparation **110-62-3P**,
Valeraldehyde 1576-86-9DP, cis-2-Pental, substituted
1576-86-9P, cis-2-Pental 1576-87-0DP, trans-2-Pental, substituted
1576-87-0P, trans-2-Pental 2100-17-6DP, 4-Pental, substituted
2100-17-6P, 4-Pental 53448-06-9DP, cis-3-Pental, substituted
53448-06-9P, cis-3-Pental 58838-14-5DP, substituted 58838-14-5P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of alkenols by reductive hydroformylation of alkadienes)
- IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0,
Triphenylphosphine, uses 607-01-2, Ethyldiphenylphosphine 1038-95-5,
Tris(p-tolyl)phosphine 1605-53-4, Diethylphenylphosphine 4023-53-4,
Tris(2-cyanoethyl)phosphine 4706-17-6, Tris(3-hydroxypropyl)phosphine
4731-53-7, Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine
6737-42-4 10210-68-1, Dicobalt octacarbonyl **12150-46-8**
14874-82-9, **Rhodium** dicarbonylacetylacetonate 17005-57-1
19262-01-2 32305-98-9D, **rhodium** complex 32376-20-8,
tert-Butyldiethylphosphine 50420-43-4 53111-20-9 60576-58-1
61806-56-2 **84680-96-6** 108793-33-5 121627-17-6 138776-88-2
138776-89-3 154813-98-6 198475-94-4
RL: CAT (Catalyst use); USES (Uses)
(preparation of alkenols by reductive hydroformylation of alkadienes)
- IT 764-37-4DP, trans-3-Penten-1-ol, substituted 764-37-4P,
trans-3-Penten-1-ol 764-38-5DP, cis-3-Penten-1-ol, substituted
764-38-5P, cis-3-Penten-1-ol 821-09-0DP, 4-Penten-1-ol, substituted
821-09-0P, 4-Pentenol 1576-95-0DP, cis-2-Penten-1-ol, substituted
1576-95-0P, cis-2-Penten-1-ol 1576-96-1DP, trans-2-Penten-1-ol,
substituted 1576-96-1P, trans-2-Penten-1-ol 77035-93-9P, 3-Pentenol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of alkenols by reductive hydroformylation of alkadienes)
- IT 106-99-0, Butadiene, reactions 106-99-0D, Butadiene, substituted
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of alkenols by reductive hydroformylation of alkadienes)
- IT **110-62-3P**, **Valeraldehyde**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of alkenols by reductive hydroformylation of alkadienes)
- RN 110-62-3 HCAPLUS
- CN Pentanal (9CI) (CA INDEX NAME)

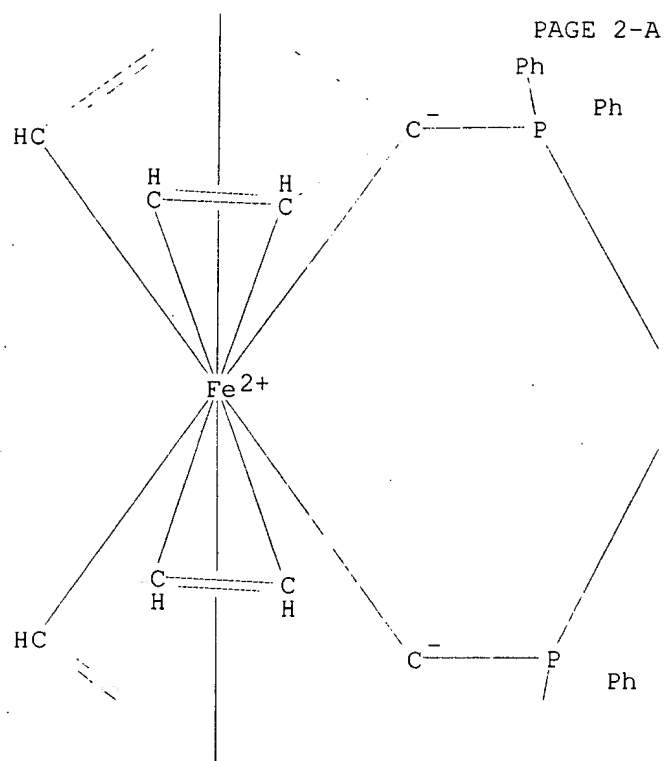


IT 12150-46-8 84680-96-6
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of alkenols by reductive hydroformylation of alkadienes)
 RN 12150-46-8 HCAPLUS
 CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)

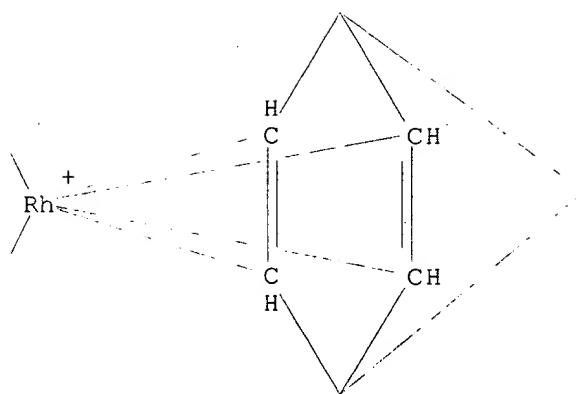


RN 84680-96-6 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)
 CM 1
 CRN 79790-97-9
 CMF C41 H36 Fe P2 Rh
 CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A

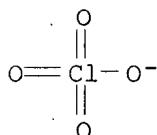
Ph

C
H

CM 2

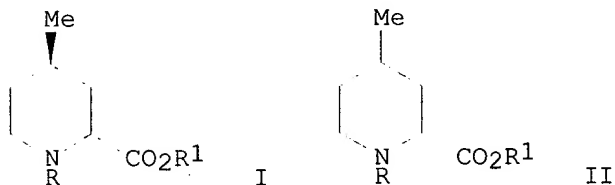
CRN 14797-73-0

CMF Cl 04



L104 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:733038 HCAPLUS
 DN 127:358790
 ED Entered STN: 21 Nov 1997
 TI New method for preparing 2,4-trans-disubstituted piperidine derivatives
 IN Grell, Wolfgang
 PA Grell, Wolfgang, Germany
 SO Ger. Offen., 30 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC ICM C07D211-60
 ICS C07B053-00
 ICA C07D211-78; B01J031-24; B01J031-22
 ICI C07M007-00; B01J023-46, B01J105-12
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19616049	A1	19971030	DE 1996-19616049	19960423 <--
PRAI	DE 1996-19616049		19960423	<--	
OS	CASREACT 127:358790; MARPAT 127:358790				
GI					



AB Piperidines I [R = H, protective group; R1 = H, alkyl, protective group] were prepared by **hydrogenation** of tetrahydropyridines II [R =

protective group; R1 = alkyl, protective group] in presence of a Rh or Ru catalyst. Thus, PhCHMeN:CHCO₂Et was cyclized with isoprene to give II [R = CHMePh, R1 = Et] which was **hydrogenated** over **rhodium**(I) [1,4-bis(diphenylphosphino)butane]-1c,5c-cyclooctadiene tetrafluoroborate followed by hydrogenolysis over Pd-C to give (2R,4R)-I [R = H, R1 = Et] with 93.6% de.

ST tetrahydropyridine stereoselective **hydrogenation** catalysts;
piperidine disubstituted stereoselective prepn

IT **Hydrogenation catalysts**

(stereoselective; preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 7440-05-3, Palladium, uses 7440-16-6, Rhodium, uses
12122-73-5 12257-42-0 12279-09-3 14694-95-2,
Tris(triphenylphosphine)**rhodium** chloride 15529-49-4
32761-50-5 32799-32-9 32965-49-4 35138-22-8 60576-58-1
62827-87-6 65012-74-0 79255-71-3 **84680-96-6** 126420-28-8
128363-26-8 130004-33-0 145926-28-9 198641-64-4

RL: CAT (Catalyst use); USES (Uses)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 78-79-5, reactions 100-46-9, Benzylamine, reactions **924-44-7**,
Ethyl glyoxylate 2627-86-3, (S)-1-Phenylethylamine 35823-28-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 37662-06-9P 127897-25-0P 139334-63-7P 145774-82-9P 198641-56-4P
198641-60-0P 198641-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 74892-82-3P 78306-52-2P 79199-61-4P 139359-60-7P 145774-81-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT **84680-96-6**

RL: CAT (Catalyst use); USES (Uses)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

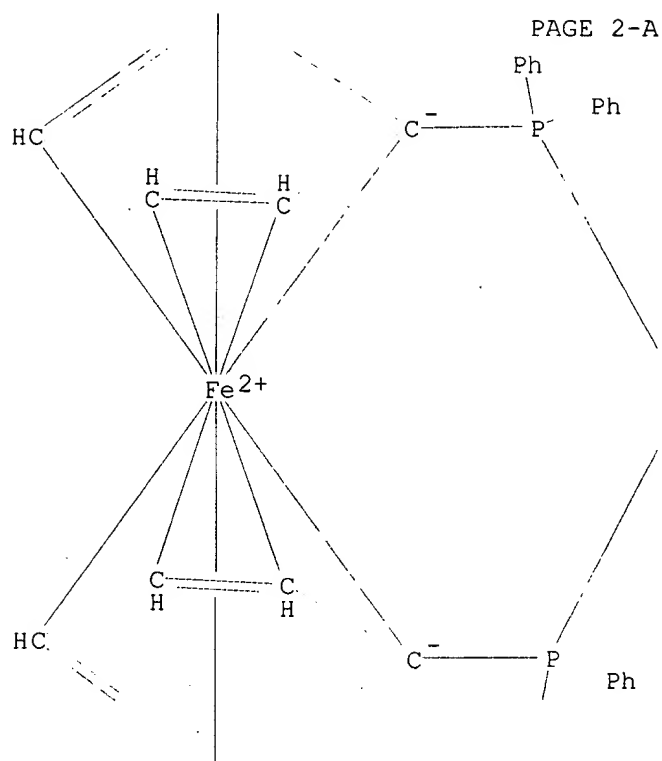
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CRN 79790-97-9

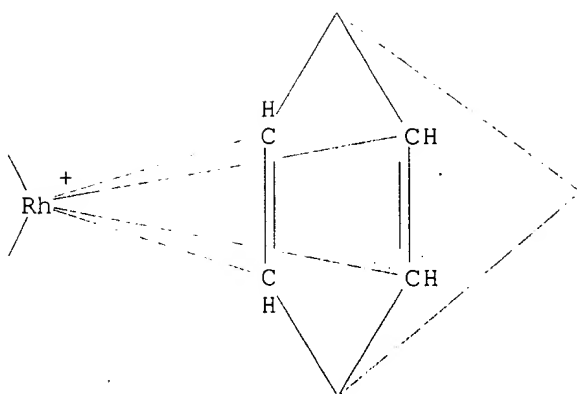
CMF C41 H36 Fe P2 Rh

CCI CCS

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PAGE 2-B



PAGE 3-A

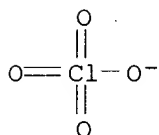
Ph

C
H

CM 2

CRN 14797-73-0

CMF C1 04



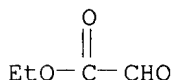
IT 924-44-7, Ethyl glyoxylate

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

RN 924-44-7 HCAPLUS

CN Acetic acid, oxo-, ethyl ester (9CI) (CA INDEX NAME)



L104 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:57590 HCAPLUS

DN 126:144405

ED Entered STN: 27 Jan 1997

TI Group 9 metal 1,1'-bis(phosphino)ferrocene complexes: synthesis, structures, solution conformation and unusual reactivity

AU Avent, Anthony G.; Bedford, Robin B.; Chaloner, Penny A.; Dewa, Shaliza Z.; Hitchcock, Peter B.

CS School Chem. and Molecular Sciences, Univ. Sussex, Brighton, BN1 9QJ, UK

SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (24), 4633-4638

CODEN: JCDBTI; ISSN: 0300-9246

PB Royal Society of Chemistry

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

AB The crystal structure of [Ir(cod)(L-L)]⁺ (3) [cod = cycloocta-1,5-diene, L-L = 1-(diisopropylphosphino)-1'-(diphenylphosphino)ferrocene] can be related to those of the analogous complexes with L-L = 1,1'-bis(diphenylphosphino)ferrocene (dppf) 1 and 1,1'-bis(diisopropylphosphino)ferrocene (disopppf), 2, all the complexes being readily synthesized from [Ir(cod)(py)₂]⁺ (py = pyridine). An optimum diphosphine bite angle of .apprx.99° is maintained in all three

complexes by varying the twist of the ferrocene, which decreases with increasing steric profile of the phosphine, and by distortion of the geometry at the Ir atom away from square planar towards tetrahedral. The twist about the ferrocene moiety induces chirality at the Ir atom in all three complexes and the interchange of stereoisomers can be followed by variable-temperature ^1H NMR spectroscopy. Application of the Eyring equation gave approx. values of ΔG^\ddagger for this process of 36.1 ± 0.2 , 39.3 ± 0.2 and 34.3 ± 0.2 kJ mol $^{-1}$ for 1-3 resp. The ligand disopfp also induces considerable distortion away from square-planar geometry in [Rh(nbd)(disopfp)][BF $_4$] (4) (nbd = norbornadiene (bicyclo[2.2.1]hepta-2,5-diene)), as found in a crystal structure

determination,

which may account for the unusual lability of the chelating diphosphine. This is demonstrated by its reactions with Ph $_2$ P(CH $_2$) $_n$ PPh $_2$ (n = 1 or 2) both of which give [Rh(L-L) $_2$] $^+$. More surprisingly, considering its lability in [Rh(nbd)(dppf)] $^+$, dppf also readily displaced disopfp from 4, to give [Rh(nbd)(dppf)][BF $_4$] (5). The nbd ligand in this complex is not displaced by reaction with an excess of dppf.

ST crystal structure iridium **rhodium** bisphosphinoferrocene diene;
mol structure iridium **rhodium** bisphosphinoferrocene diene;
kinetics conformational inversion iridium bisphosphinoferrocene diene;
bisphosphinoferrocene iridium **rhodium** complex prepn structure;
ferrocene bisphosphino iridium **rhodium** complex prepn;
coordinative substitution **rhodium** bisphosphinoferrocene diene complex

IT Crystal structure

Molecular structure

(of iridium and **rhodium** diene bisphosphinoferrocene complexes)

IT Conformational transition

(of iridium bisphosphinoferrocene diene complexes)

IT Substitution reaction, coordinative

(of **rhodium** diene bisphosphinoferrocene complex)

IT 56678-60-5, (1,5-Cyclooctadiene)bis(pyridine)iridium(1+)
hexafluorophosphate

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution reactions with bisphosphinoferrocenes)

IT 97239-80-0, 1,1'-Bis(diisopropylphosphino)ferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution reactions with iridium and **rhodium** diene complexes)

IT 36620-11-8, Bis(norbornadiene)**rhodium**(1+) tetrafluoroborate

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with bis(diisopropylphosphino)ferrocene)

IT 97239-85-5, 1-Diisopropylphosphino-1'-diphenylphosphinoferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with iridium COD pyridine complex)

IT 1663-45-2, 1,2-Bis(diphenylphosphino)ethane 2071-20-7,

Bis(diphenylphosphino)methane 12150-46-8, 1,1'-

Bis(diphenylphosphino)ferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with **rhodium**

bis(diisopropylphosphino)ferrocene diene complex)

IT 53450-77-4P, Bis(bis(diphenylphosphino)methane)**rhodium**(1+)

53450-79-6P, Bis(1,2-bis(diphenylphosphino)ethane)**rhodium**(1+)

tetrafluoroborate 79790-98-0P, (1,1'-

Bis(diphenylphosphino)ferrocene) (norbornadiene)**rhodium**(1+)

tetrafluoroborate

RL: SPN (Synthetic preparation); PREP (Preparation)

(formation by coordinative substitution with

bis(diisopropylphosphino)ferrocene analog)

IT 151705-16-7, (1,1'-Bis(diphenylphosphino)ferrocene) (1,5-

cyclooctadiene)iridium(1+) hexafluorophosphate

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(kinetics of conformational inversion and comparison to other bisphosphinoferrocene complexes)

IT 186692-55-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coordinative substitution reactions with diphosphines)

IT 186692-56-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

IT 167545-45-1P, (1,1'-Bis(diisopropylphosphino)ferrocene) (1,5-cyclooctadiene)iridium(1+) tetraphenylborate

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

IT 186692-54-6P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, crystal structure and kinetics of conformational inversion of)

IT 167545-42-8P, (1,1'-Bis(diisopropylphosphino)ferrocene) (1,5-cyclooctadiene)iridium(1+) hexafluorophosphate

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, metathesis and kinetics of conformational inversion of)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(23) Sheldrick, G; SHELXL 93 1993

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(25) Uson, R; Transition Met Chem 1979, V4, P55 HCAPLUS

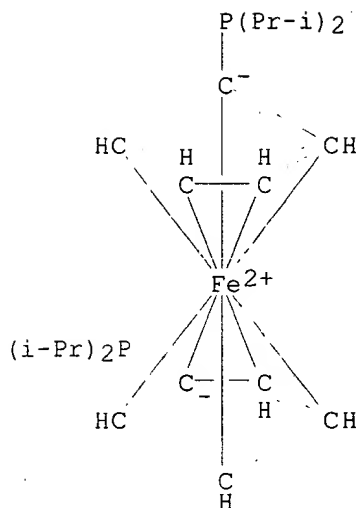
IT 97239-80-0, 1,1'-Bis(diisopropylphosphino)ferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

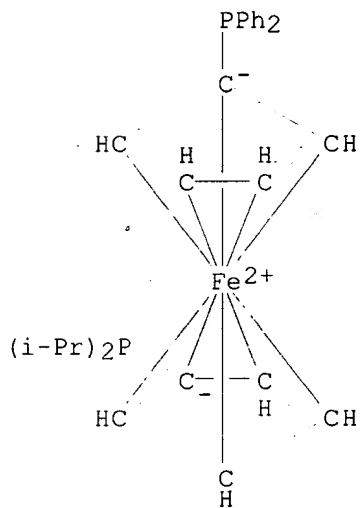
(coordinative substitution reactions with iridium and rhodium diene complexes)

RN 97239-80-0 HCAPLUS

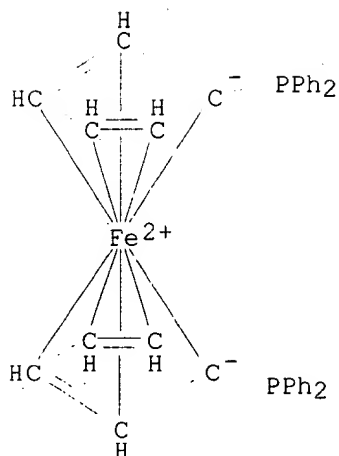
CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



IT 97239-85-5, 1-Diisopropylphosphino-1'-diphenylphosphinoferrocene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (coordinative substitution with iridium COD pyridine complex)
 RN 97239-85-5 HCAPLUS
 CN Ferrocene, 1-[bis(1-methylethyl)phosphino]-1'-(diphenylphosphino)- (9CI)
 (CA INDEX NAME)



IT 12150-46-8, 1,1'-Bis(diphenylphosphino)ferrocene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (coordinative substitution with **rhodium**
 bis(diisopropylphosphino)ferrocene diene complex)
 RN 12150-46-8 HCAPLUS
 CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



IT 79790-98-0P, (1,1'-Bis(diphenylphosphino)ferrocene) (norbornadiene)
 rhodium(1+) tetrafluoroborate
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (formation by coordinative substitution with
 bis(diisopropylphosphino)ferrocene analog)
 RN 79790-98-0 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
 bis(diphenylphosphino- κ P)ferrocene]-, tetrafluoroborate(1-) (9CI)
 (CA INDEX NAME)

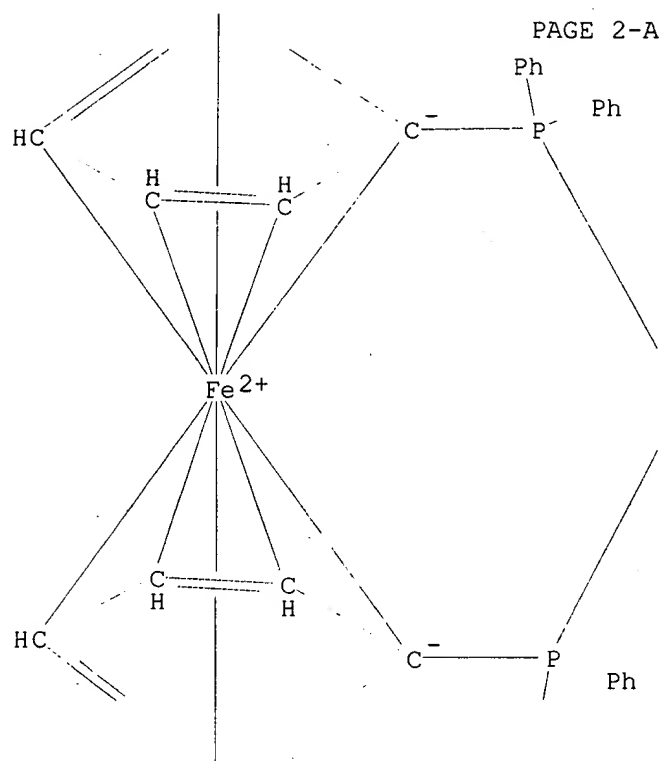
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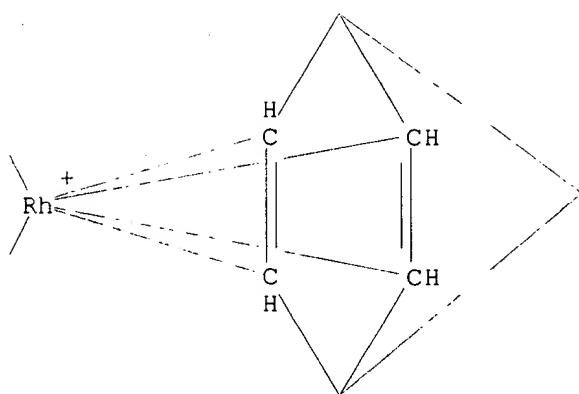
CMF C41 H36 Fe P2 Rh

CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A

Ph

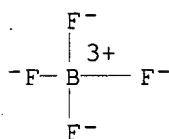
C
H

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 151705-16-7, (1,1'-Bis(diphenylphosphino)ferrocene) (1,5-cyclooctadiene)iridium(1+) hexafluorophosphate
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
 (kinetics of conformational inversion and comparison to other bisphosphinoferrocene complexes)

RN 151705-16-7 HCAPLUS

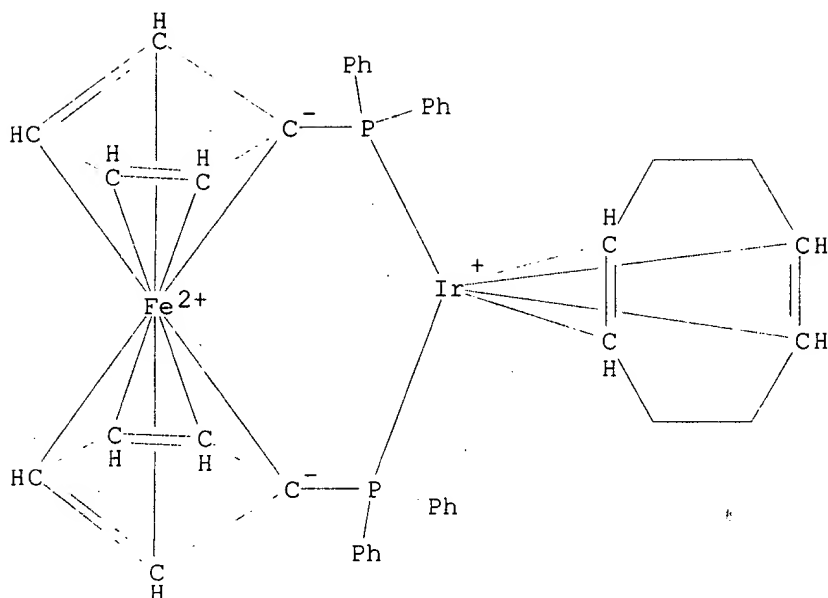
CN Iridium(1+), [1,1'-bis(diphenylphosphino-κP)ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 112947-50-9

CMF C42 H40 Fe Ir P2

CCI CCS

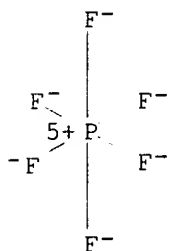


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 186692-55-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coordinative substitution reactions with diphosphines)

RN 186692-55-7 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene]-, tetrafluoroborate(1-)
(9CI) (CA INDEX NAME)

CM 1

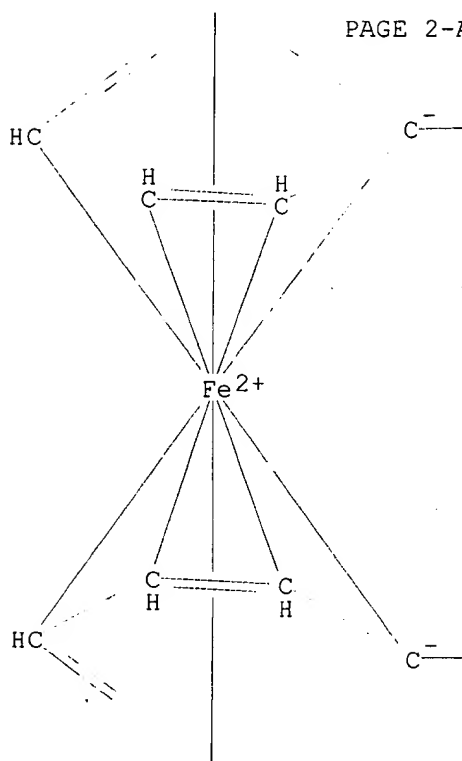
CRN 96144-62-6

CMF C29 H44 Fe P2 Rh

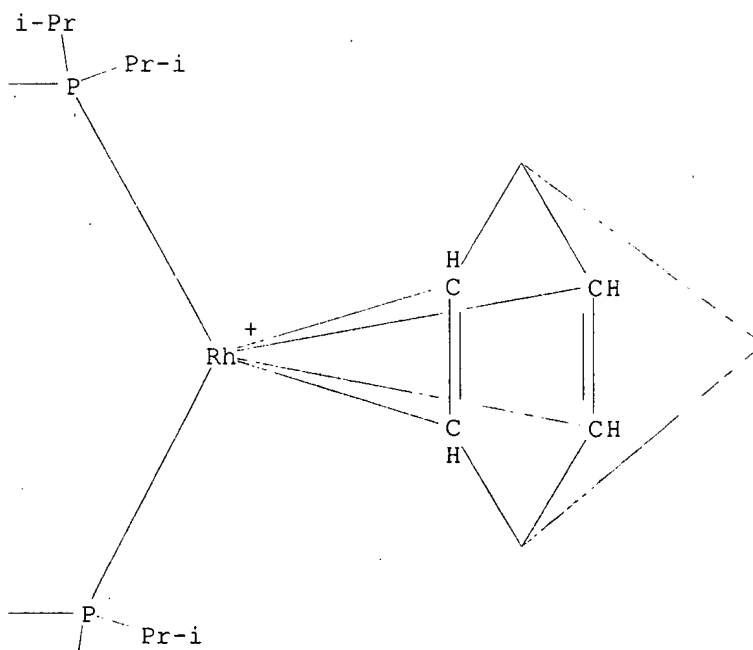
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
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PAGE 3-B

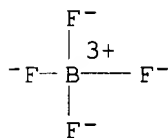
i-Pr

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 186692-56-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

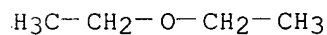
RN 186692-56-8 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene]-, tetrafluoroborate(1-), compd. with 1,1'-oxybis[ethane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 60-29-7

CMF C4 H10 O



CM 2

CRN 186692-55-7

CMF C29 H44 Fe P2 Rh . B F4

CM 3

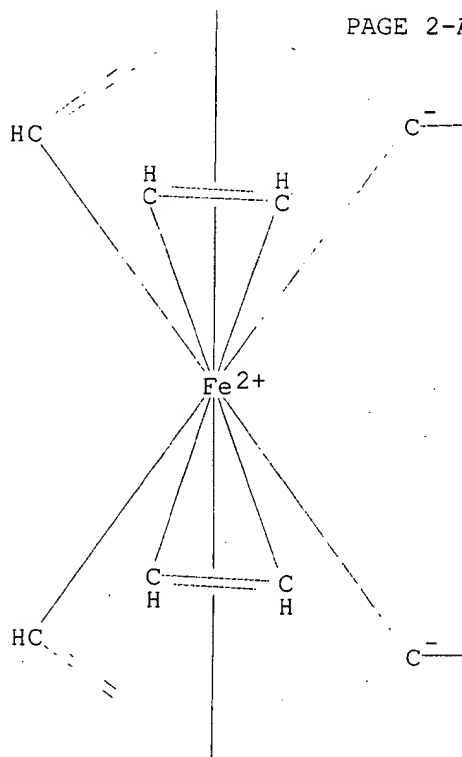
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CMF C29 H44 Fe P2 Rh

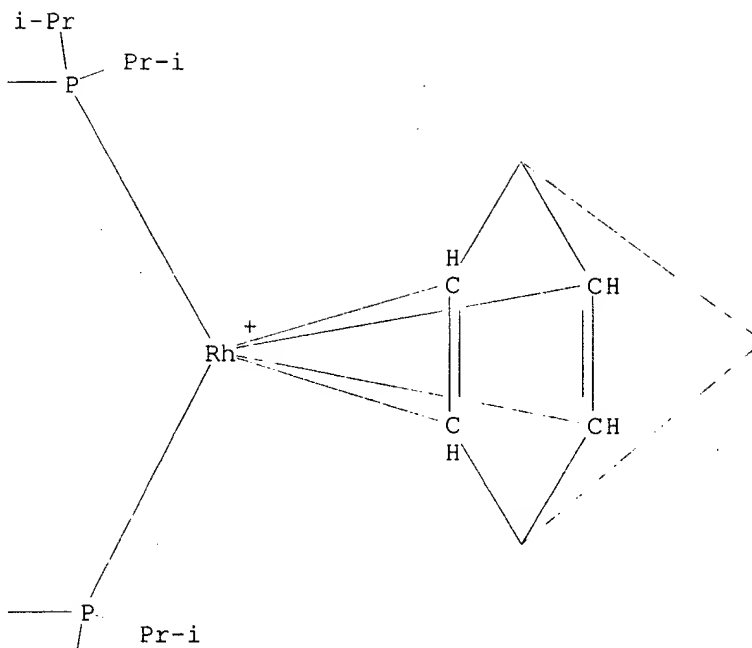
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
H

PAGE 3-B

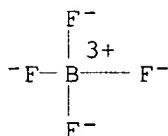
i-Pr

CM 4

CRN 14874-70-5

CMF B F4

CCI CCS



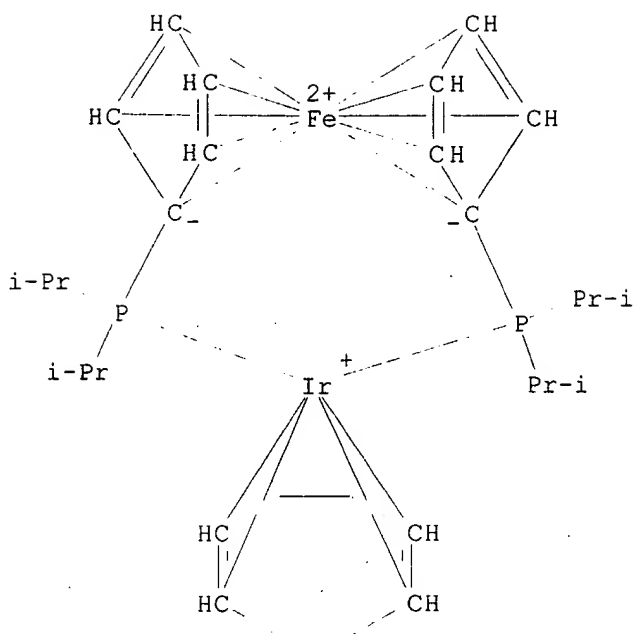
IT 167545-45-1P, (1,1'-Bis(diisopropylphosphino)ferrocene) (1,5-cyclooctadiene)iridium(1+) tetraphenylborate
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 167545-45-1 HCAPLUS
 CN Iridium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 167545-41-7

CMF C30 H48 Fe Ir P2

CCI CCS

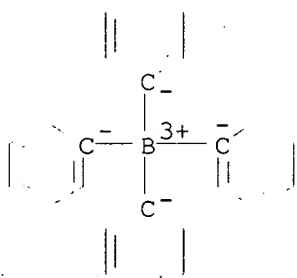


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



IT 186692-54-6P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, crystal structure and kinetics of conformational inversion of)

RN 186692-54-6 HCAPLUS

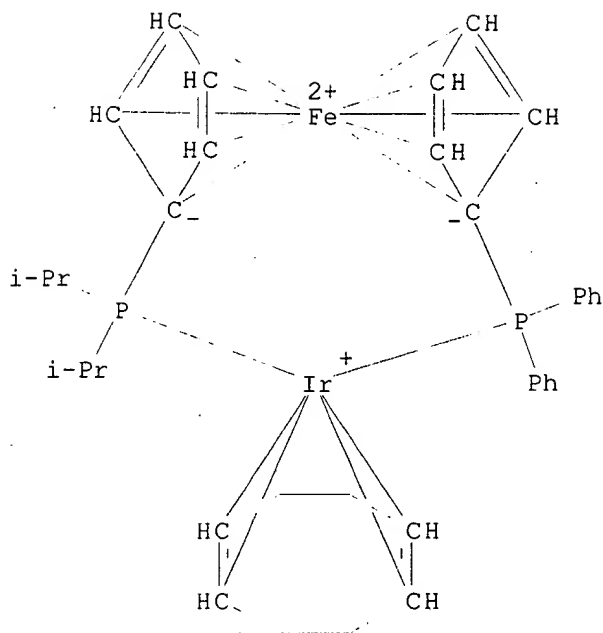
CN Iridium(1+), [1-[bis(1-methylethyl)phosphino-κP]-1'-(diphenylphosphino-κP)ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 186692-53-5

CMF C36 H44 Fe Ir P2

CCI CCS

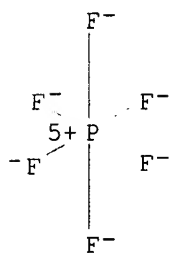


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



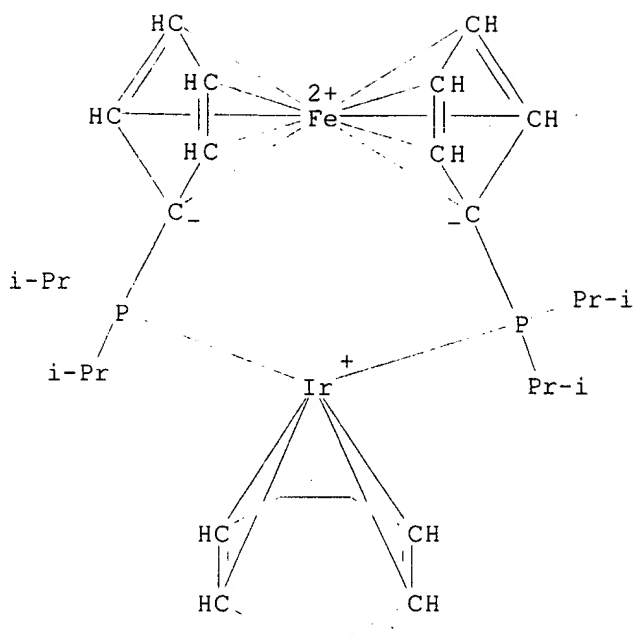
IT **167545-42-8P**, (1,1'-Bis(diisopropylphosphino)ferrocene) (1,5-cyclooctadiene)iridium(1+) hexafluorophosphate
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (preparation, metathesis and kinetics of conformational inversion of)
 RN 167545-42-8 HCAPLUS
 CN Iridium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 167545-41-7

CMF C30 H48 Fe Ir P2

CCI CCS

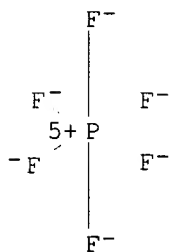


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



L104 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:1004413 HCAPLUS

DN 124:116619

ED Entered STN: 26 Dec 1995

TI Catalytic cyclization of some alkynes by rhodium and iridium complexes of ferrocene-containing ligands

AU Kim, Tae-Jeong; Kim, So-Hoon; Shim, Sang-Chul; Jeong, Jong-Hwa

CS Dep. of Industrial Chemistry, Kyungpook National Univ., Taegu, 702-701, S. Korea

SO Bulletin of the Korean Chemical Society (1995), 16(11), 1126-8

CODEN: BKCSDE; ISSN: 0253-2964

PB Korean Chemical Society

DT Journal

LA English

CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 29, 75

OS CASREACT 124:116619

AB The lactonization of 4-pentynoic acid and the cocyclotrimerization of N-benzylpropargylamine with PhC.tplbond.CH, both reaction catalyzed by Rh and Ir complexes with ferrocenylphosphines and -imines, were studied. [(COD)Ir(PPFA)]ClO₄ (PPFA = 2-diphenylphosphino-1-(N,N-dimethylaminoethyl)ferrocene) was prepared and its crystal structure determined

ST crystal structure iridium aminoethylphosphinoferrocene; aminoethylphosphinoferrocene iridium prepn structure; cyclization catalyst iridium rhodium phosphinoferrocene alkyne

IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic cyclization in presence of iridium and rhodium phosphinoferrocene complexes)

IT Ring closure catalysts
(iridium and rhodium phosphinoferrocene complexes for alkynes)

IT 536-74-3, Phenylacetylene 1197-51-9 6089-09-4, 4-Pentynoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic cyclization in presence of iridium and rhodium phosphinoferrocene complexes)

IT 91159-10-3 112947-51-0 125939-72-2 173101-24-1 173101-26-3
173101-28-5 173967-26-5
RL: CAT (Catalyst use); USES (Uses)
(cyclization catalysts for alkynes)

IT 12112-67-3, Dichlorobis(cyclooctadiene)diiridium 105088-01-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of iridium cyclooctadiene aminoethylphosphinoferrocene complex)

IT 173101-31-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

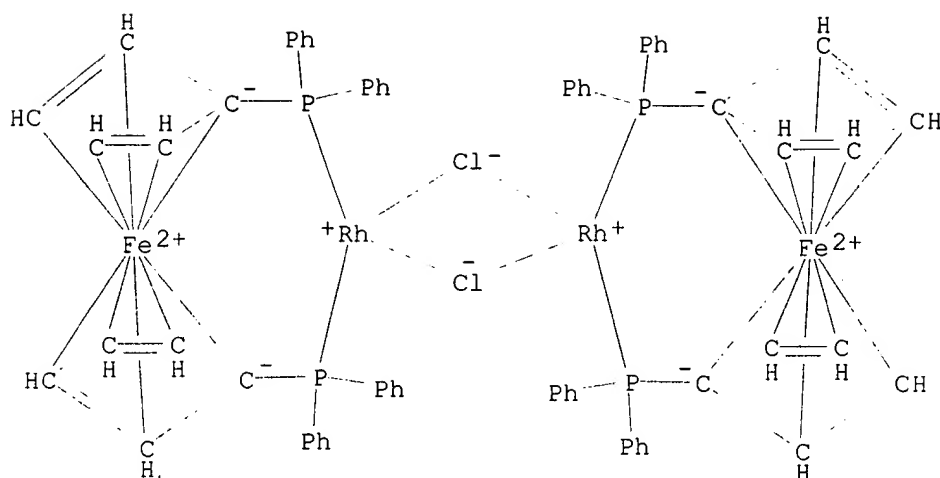
IT 173101-30-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

IT 10008-73-8P 173101-22-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation by catalytic cyclization of alkynes in presence of iridium and rhodium phosphinoferrocene complexes)

IT 125939-72-2
RL: CAT (Catalyst use); USES (Uses)
(cyclization catalysts for alkynes)

RN 125939-72-2 HCAPLUS

CN Rhodium, bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di-μ-chlorodi-
(9CI) (CA INDEX NAME)



L104 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:578803 HCAPLUS

DN 121:178803

ED Entered STN: 15 Oct 1994

TI Efficient **rhodium**-catalyzed **hydrogenation** of **aldehydes** and ketones

AU **Burk, Mark J.**; Harper, T. Gregory P.; Lee, Jeffrey R.; Kalberg, Christopher

CS Dep. Chem., Duke Univ., Durham, NC, 27706, USA

SO Tetrahedron Letters (1994), 35(28), 4963-6

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

CC 21-2 (General Organic Chemistry)

OS CASREACT 121:178803

AB A cationic **rhodium**(I) catalyst bearing the air-stable and crystalline diphosphine 1,1'-bis(diisopropylphosphino)ferrocene allows the **hydrogenation** of **aldehydes** and ketones under mild conditions.

ST **rhodium** ferrocene catalyst **hydrogenation** carbonyl;
aldehyde hydrogenation rhodium catalyst;
ketone **hydrogenation rhodium** catalyst

IT **Aldehydes, reactions**

Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(**hydrogenation** of, **rhodium** ferrocene complex as catalyst for)

IT **Hydrogenation catalysts**

(**rhodium** ferrocene complex, for **aldehydes** and ketones)

IT 97239-80-0

RL: CAT (Catalyst use); USES (Uses)

(catalysts, containing bis(cyclooctadiene)**rhodium** triflate, for **hydrogenation** of **aldehydes** and ketones)

IT 99326-34-8

RL: CAT (Catalyst use); USES (Uses)

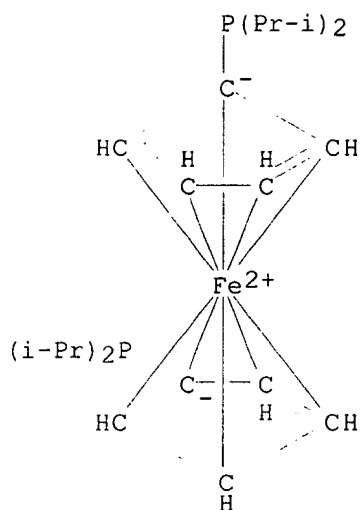
(catalysts, containing bis(diisopropylphosphino)ferrocene, for **hydrogenation** of **aldehydes** and ketones)

IT 157772-66-2

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for **hydrogenation** of **aldehydes** and ketones)

- IT 66-25-1, Hexanal 78-93-3, 2-Butanone, reactions 98-01-1
 , 2-Furancarboxaldehyde, reactions 98-03-3, 2-
Thiophenecarboxaldehyde 98-53-3 98-86-2, Acetophenone,
 reactions 100-52-7, **Benzaldehyde**, reactions
 108-94-1, Cyclohexanone, reactions 119-53-9, Benzoin 122-57-6,
 Benzalacetone 372-31-6 434-45-7, Trifluoroacetophenone 513-86-0
 609-38-1, 2-Furancarboxamide 630-19-3, **Pivalaldehyde**
 1603-79-8, Ethyl oxophenylacetate 1694-31-1, tert-Butyl 3-oxobutanoate
 3524-62-7 3891-59-6 7152-15-0, Pentanoic acid, 4-methyl-3-oxo-, ethyl
 ester 20201-24-5, Butanoic acid, 3-methyl-2-oxo-, ethyl ester
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of, rhodium ferrocene complex as
 catalyst for)
- IT 2550-26-7P, 4-Phenyl-2-butanone
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrogenation of, rhodium ferrocene
 complex as catalyst for)
- IT 2344-70-9P, 4-Phenyl-2-butanol
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- IT 100-51-6P, Benzyl alcohol, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by rhodium complex-catalyzed
 hydrogenation of benzaldehyde)
- IT 579-43-1P 655-48-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by rhodium complex-catalyzed
 hydrogenation of benzoin)
- IT 5341-95-7P 6982-25-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by rhodium complex-catalyzed
 hydrogenation of hydroxybutanone)
- IT 937-05-3P, Cyclohexanol, 4-(1,1-dimethylethyl)-, cis- 21862-63-5P,
 Cyclohexanol, 4-(1,1-dimethylethyl)-, trans-
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by rhodium complex-catalyzed
 hydrogenation of ketone)
- IT 97239-80-0
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, containing bis(cyclooctadiene)rhodium triflate, for
 hydrogenation of aldehydes and ketones)
- RN 97239-80-0 HCAPLUS
- CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



IT 157772-66-2

RL: CAT (Catalyst use); USES (Uses)
(catalysts, for **hydrogenation** of **aldehydes** and **ketones**)

RN 157772-66-2 HCAPLUS

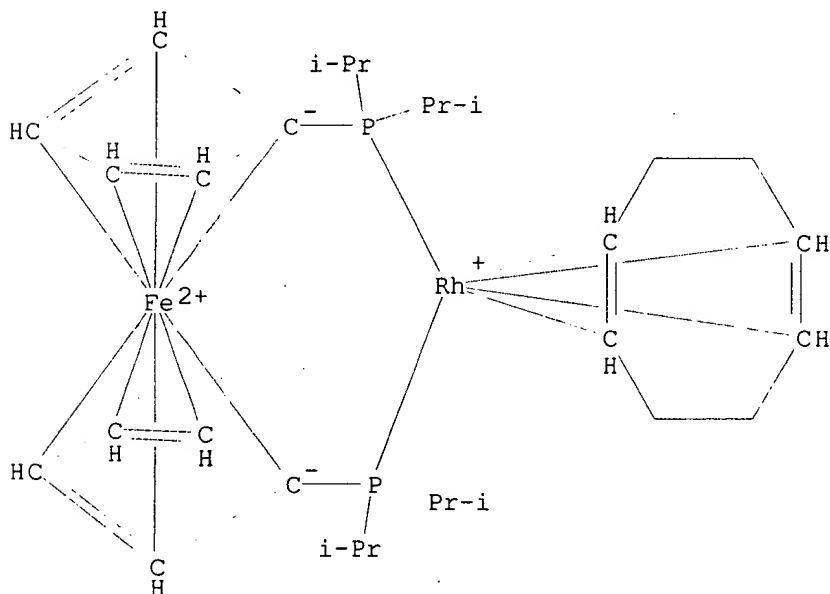
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-
P,P'][(1,2,5,6- η)-1,5-cyclooctadiene]-, salt with
trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 157772-65-1

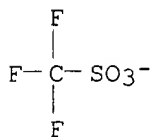
CMF C30 H48 Fe P2 Rh

CCI CCS



CM 2

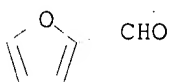
CRN 37181-39-8
CMF C F3 O3 S



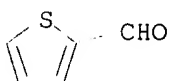
IT 66-25-1, Hexanal 98-01-1, 2-Furancarboxaldehyde
, reactions 98-03-3, 2-Thiophenecarboxaldehyde
100-52-7, Benzaldehyde, reactions 630-19-3,
Pivalaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, rhodium ferrocene complex as
catalyst for)
RN 66-25-1 HCAPLUS
CN Hexanal (8CI, 9CI) (CA INDEX NAME)

OHC-(CH₂)₄-Me

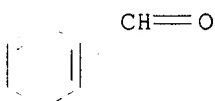
RN 98-01-1 HCAPLUS
CN 2-Furancarboxaldehyde (9CI) (CA INDEX NAME)



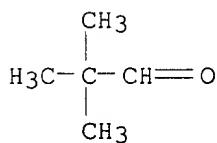
RN 98-03-3 HCAPLUS
CN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 100-52-7 HCAPLUS
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



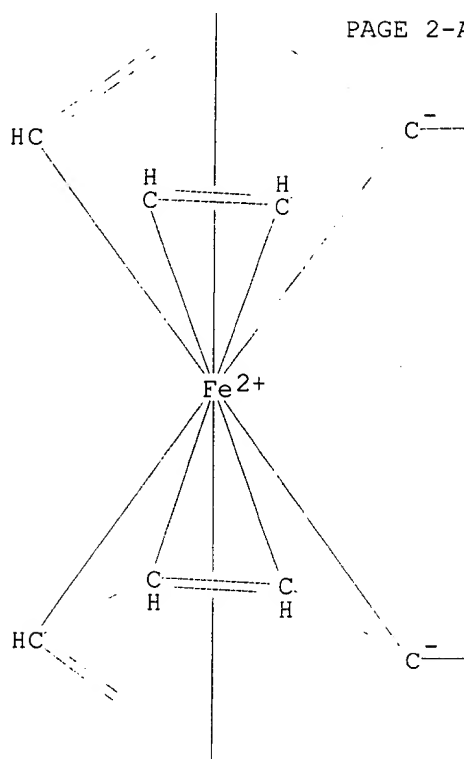
RN 630-19-3 HCAPLUS
CN Propanal, 2,2-dimethyl- (9CI) (CA INDEX NAME)



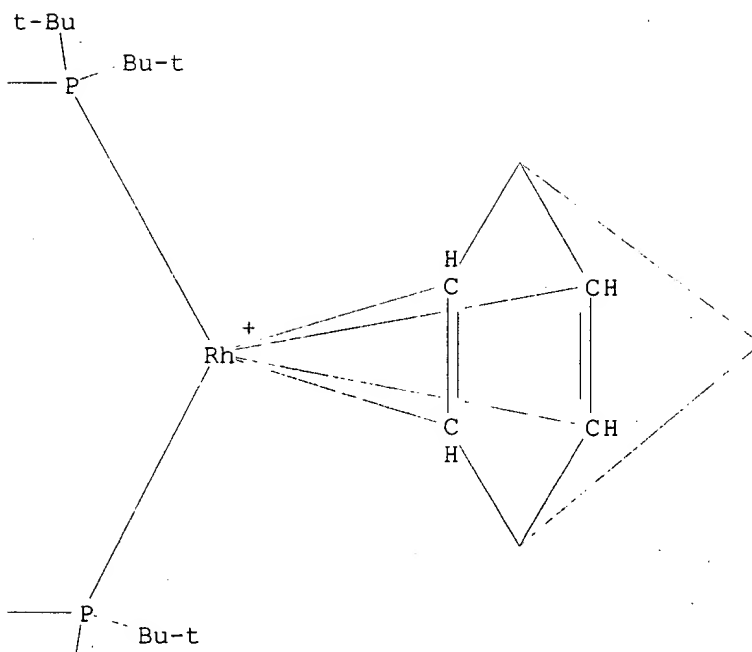
L104 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:603799 HCAPLUS
DN 113:203799
ED Entered STN: 23 Nov 1990
TI Synthesis and solution chemistry of metal hydrides from cationic
rhodium(I) catalyst precursors [(L-L)Rh(NBD)]ClO₄ (L-L =
Fe(η 5-C₅H₄PBu-tert)₂, Fe(η 5-C₅H₄PPhBu-tert)₂)
AU Kim, Tae Jeong
CS Dep. Ind. Chem., Kyungpook Natl. Univ., Taegu, 702-701, S. Korea
SO Bulletin of the Korean Chemical Society (1990), 11(2), 134-9
CODEN: BKCSDE; ISSN: 0253-2964
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 29, 77
AB The **hydrogenation** catalyst precursors [(L-L)Rh
(NBD)]ClO₄ (L-L = Fe(η 5-C₅H₄P(CMe₃)₂)₂, Fe(η 5-C₅H₄PPhCMe₃)₂; NBD =
norbornadiene) react with H₂ (1 atm, 30°, MeOH) to yield
[(L-L)HRh(μ -H)3Rh(L-L)]ClO₄. These hydrido species are fluxional, and
variable temperature NMR studies show the existence of a number of equilibrium
involving
both fluxional and nonfluxional species. The synthesis, solution structures,
and fluxional behaviors of these hydrides are described.
ST fluxionality **rhodium** hydrido ferrocenylphosphine dinuclear;
phosphine ferrocenyl **rhodium** hydrido dinuclear
IT Fluxional rearrangement
(of **rhodium** hydrido ferrocenylphosphine dinuclear complexes)
IT 84680-97-7 92284-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)
IT 92468-70-7P 130322-22-4P
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN
(Synthetic preparation); PREP (Preparation); PROC (Process); RACT
(Reactant or reagent)
(preparation and fluxionality of)
IT 84680-97-7 92284-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)
RN 84680-97-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']- (9CI) (CA INDEX
NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
H

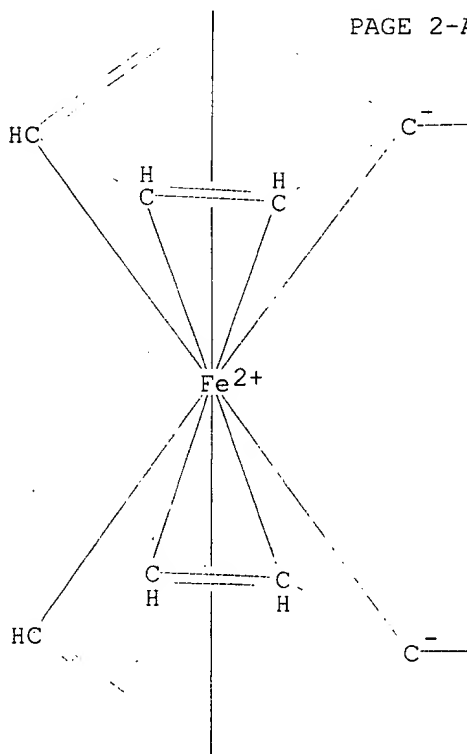
PAGE 3-B

t-Bu

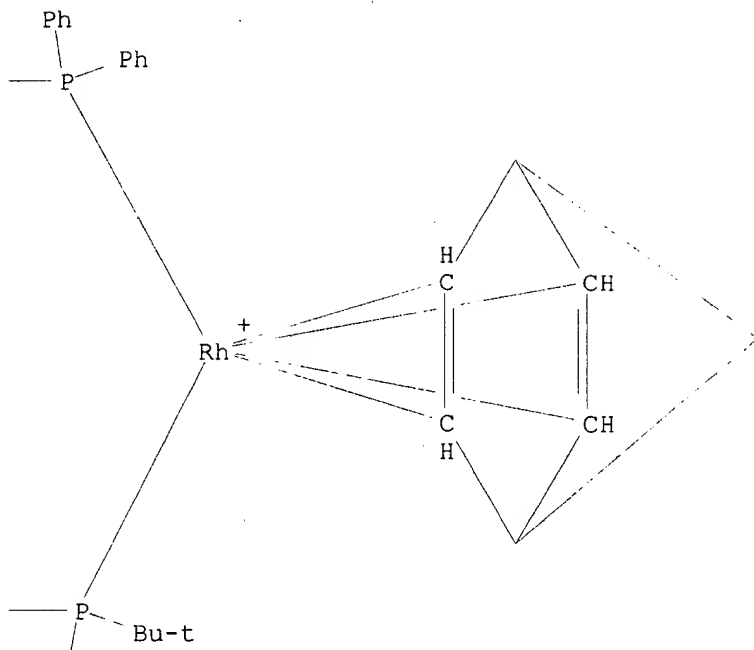
RN 92284-06-5 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']- (9CI) (CA INDEX NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



PAGE 3-B

t-Bu

IT 92468-70-7P 130322-22-4P

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation and fluxionality of)

RN 92468-70-7 HCAPLUS

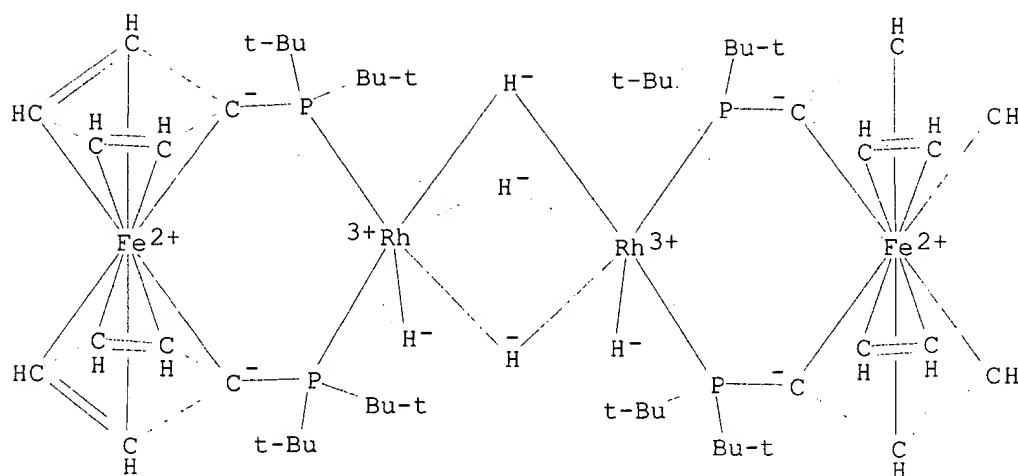
CN Rhodium(1+), bis[1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92468-69-4

CMF C52 H93 Fe2 P4 Rh2

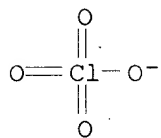
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 130322-22-4 HCAPLUS

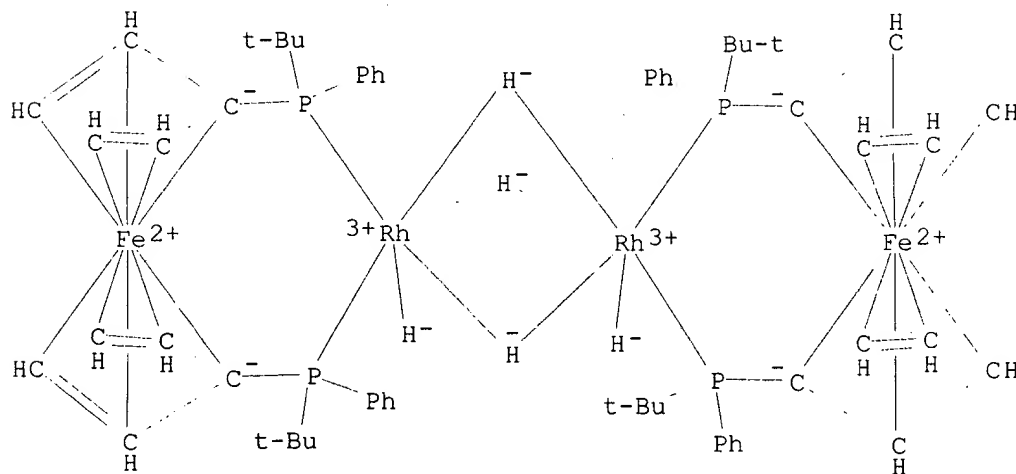
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-
P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 130322-21-3

CMF C60 H77 Fe2 P4 Rh2

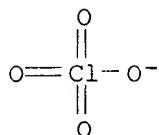
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



L104 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:139478 HCAPLUS

DN 112:139478

ED Entered STN: 13 Apr 1990

TI **Rhodium**(I) complexes of 1,1'-bis(diphenylphosphino)ferrocene as efficient catalysts in regioselective hydrogenation of polynuclear heteroaromatic compounds

AU Kim, Tae Jeong; Lee, Kyu Chul

CS Dep. Ind. Chem., Kyungpook Natl. Univ., Taegu, 702-701, S. Korea

SO Bulletin of the Korean Chemical Society (1989), 10(3), 279-82

CODEN: BKCSDE; ISSN: 0253-2964

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 27

AB Two **rhodium**(I) complexes of the types [Rh(BPPF)(NBD)]ClO₄ (I) and [Rh(BPPF)Cl]₂ (II) (BPPF = 1,1'-bis(diphenylphosphino)ferrocene, NBD = norbornadiene) were prepared and investigated as catalysts for the regioselective hydrogenation of polynuclear heteroarom. N and S compds. such as quinoline, acridine, phenanthridine, 7,8-benzoquinoline, benzothiophene, isoquinoline, indole, pyridine, and thiophene. Both complexes I and II, except for the cases of indole and mononuclear heteroaroms. pyridine and thiophene, are very efficient in the selective reduction under quite mild hydrogenation conditions to give the corresponding saturated N and S heterocyclic analogs in fast conversion rates and in excellent yields. Relative rate studies revealed that the reduction depends significantly on the steric and electronic effects of the substrates. Of the two complexes, the dimeric species II gives faster reaction rates in all cases studied.

ST phenylphosphinoferrocene **rhodium** complex regioselective hydrogenation catalyst; heterocyclic nitrogen sulfur hydrogenation catalyst; kinetics hydrogenation nitrogen sulfur heterocycle

IT **Hydrogenation catalysts**

(bis(diphenylphosphino)ferrocene **rhodium** complexes, for nitrogen and sulfur heterocycles)

IT Regiochemistry

(of hydrogenation of nitrogen and sulfur heterocycles, **rhodium** complex-catalyzed)

IT Kinetics of hydrogenation

(of nitrogen and sulfur heterocyclic compds., **rhodium**-catalyzed)

IT Heterocyclic compounds

RL: RCT (Reactant); RACT (Reactant or reagent)

(nitrogen, regioselective hydrogenation of, **rhodium** catalysts for)

IT Heterocyclic compounds

RL: RCT (Reactant); RACT (Reactant or reagent)

(sulfur, regioselective hydrogenation of, **rhodium** catalysts for)

IT 110-02-1, Thiophene 110-86-1, Pyridine, reactions 120-72-9, 1H-Indole, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (attempted hydrogenation of, **rhodium**-catalyzed)

IT 84680-96-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for regioselective hydrogenation of nitrogen and sulfur heterocycles)

IT 7727-37-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (heterocyclic compounds, nitrogen, regioselective hydrogenation of, **rhodium** catalysts for)

IT 7704-34-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (heterocyclic compounds, sulfur, regioselective hydrogenation of, **rhodium** catalysts for)

IT 91-22-5, Quinoline, reactions 95-15-8, Benzothiophene 119-65-3, Isoquinoline 229-87-8, Phenanthridine 230-27-3, 7,8-Benzoquinoline 260-94-6, Acridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of, (diphenylphosphino)**ferrocenerhodium** complex catalysts for, regiochem. and kinetics of)

IT 125939-72-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation as hydrogenation catalyst, for nitrogen and sulfur heterocycles)

IT 91-21-4P 92-81-9P 635-46-1P 4565-32-6P 5223-80-3P 27799-79-7P
 125916-39-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 12150-46-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction by, of norbornadiene **rhodium** complex)

IT 12257-42-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with bis(diphenylphosphino)ferrocene)

IT 84680-96-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for regioselective hydrogenation of nitrogen and sulfur heterocycles)

RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

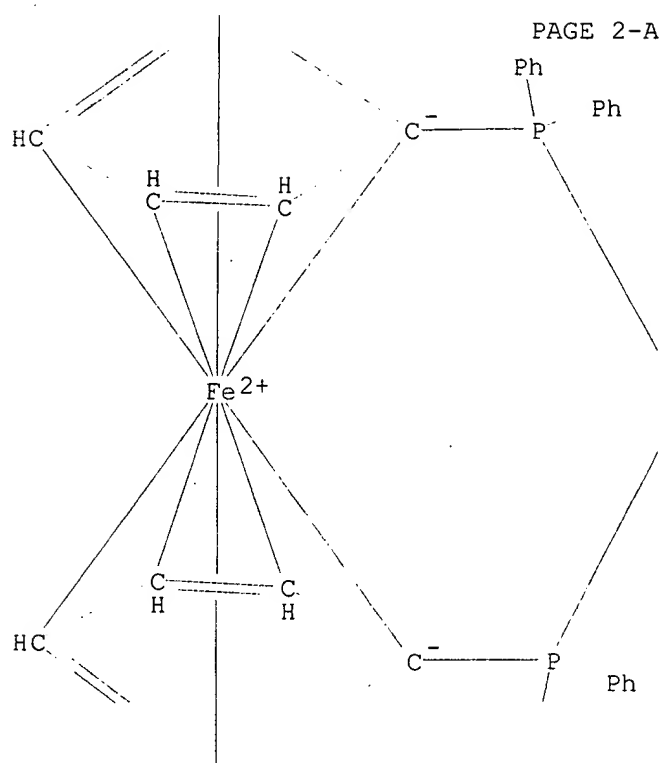
CM 1

CRN 79790-97-9

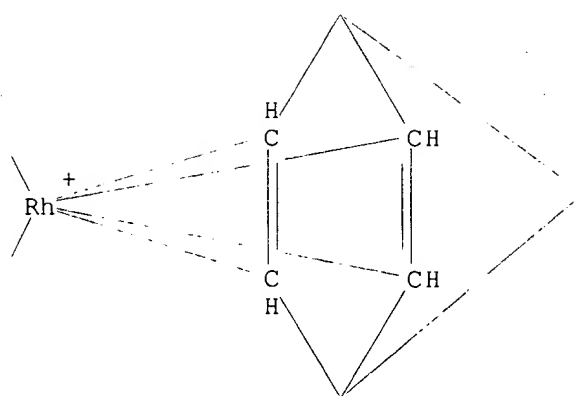
CMF C41 H36 Fe P2 Rh

CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A

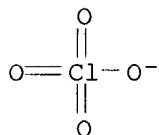
Ph



CM 2

CRN 14797-73-0

CMF Cl O4

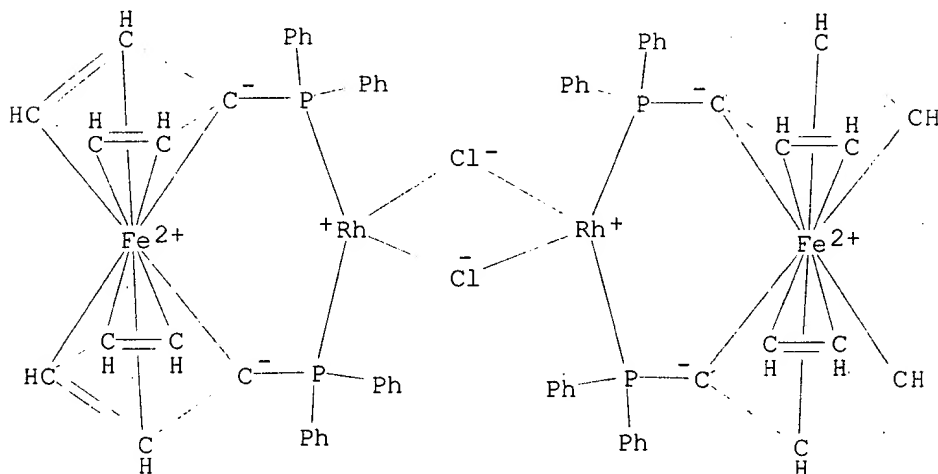


IT 125939-72-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation as hydrogenation catalyst, for nitrogen and sulfur heterocycles)

RN 125939-72-2 HCAPLUS

CN Rhodium, bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di-μ-chlorodi-
(9CI) (CA INDEX NAME)

IT 125916-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

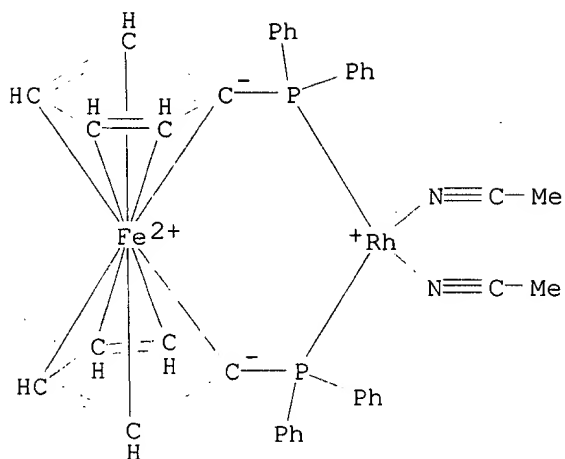
RN 125916-39-4 HCAPLUS

CN Rhodium(1+), bis(acetonitrile)[1,1'-bis(diphenylphosphino)ferrocene-P,P']-
, (SP-4-2)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

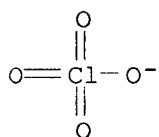
CRN 125916-38-3

CMF C38 H34 Fe N2 P2 Rh
CCI CCS



CM 2

CRN 14797-73-0
CMF C1 O4



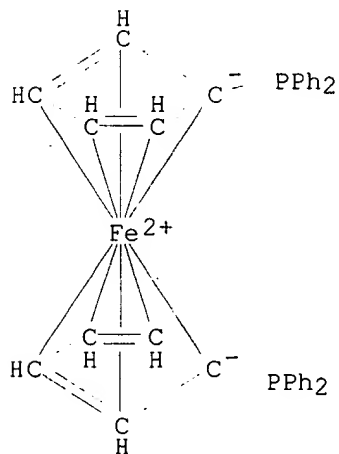
IT 12150-46-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reaction by, of norbornadiene rhodium complex)

RN 12150-46-8 HCAPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



AN 1985:471462 HCAPLUS
DN 103:71462
ED Entered STN: 07 Sep 1985
TI 1,1'-Bis(alkylarylphosphino)ferrocenes: synthesis, metal complex formation, and crystal structure of three metal complexes of $\text{Fe}(\eta^5\text{-C}_5\text{H}_4\text{PPh}_2)_2$
AU Butler, Ian R.; Cullen, William R.; Kim, Tae Jeong; Rettig, Steven J.; Trotter, James
CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SO Organometallics (1985), 4(6), 972-80
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
CC 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
OS CASREACT 103:71462
GI For diagram(s), see printed CA Issue.
AB The ferrocenylbisphosphines I ($\text{R} = \text{PR}_2\text{R}_3$; $\text{R}_1 = \text{PR}_4\text{R}_5$) ($\text{R}_2\text{-R}_5 = \text{Ph}$ or Me_3C) were prepared by treating either dilithio I ($\text{R} = \text{R}_1 = \text{Li}$) or I ($\text{R} = \text{Li}$, $\text{R}_1 = \text{PR}_4\text{R}_5$) (II) with ClPR_2R_3 . II was obtained by cleaving ferrocenophane I ($\text{RR}_1 = \text{PR}_4$) with R_5Li . Best results were obtained when R_4 and/or $\text{R}_5 = \text{Ph}$. A range of PdLCl_2 , NiLX_2 , and $[\text{Rh}(\text{L})(\text{NBD})]\text{ClO}_4$ [$\text{L} = \text{I}$; $\text{R}_1, \text{R}_2 = \text{PPh}_2$, $\text{P}(\text{CMe}_3)_2$, PPhCMe_3 ; $\text{NBD} = \text{norbornadiene}$; $\text{X} = \text{Cl}, \text{Br}$] complexes were prepared. The crystal structures of PdLCl_2 , NiLBr_2 , and $\text{MoL}(\text{CO})_4$ ($\text{L} = \text{I}$; $\text{R} = \text{R}_1 = \text{PPh}_2$) showed the metal atoms had cis-square planar, tetrahedral, and cis-octahedral coordination, resp. The I ($\text{R} = \text{R}_1 = \text{PPh}_2$) ligands have slightly nonparallel cyclopentadienyl rings, with approx. staggered arrangements in the Pd and Mo compds. but an approx. eclipsed conformation in the Ni complex, with significant displacements of the P atoms from the ring planes. $\text{ML}(\text{CO})_4$ ($\text{M} = \text{Mo}, \text{Cr}$; $\text{L} = \text{I}$; $\text{R} = \text{R}_1 = \text{PPh}_2$) are fluxional in solution to -80° .
ST crystal structure ferrocenyl bisphosphine metal complex; mol structure ferrocenyl bisphosphine metal complex; phosphinoferrocene metal complex crystal structure; molybdenum bisphosphinoferrocene complex crystal structure; palladium bisphosphinoferrocene complex crystal structure; nickel bisphosphinoferrocene complex crystal structure; fluxionality chromium molybdenum bisphosphinoferrocene complex
IT Crystal structure
Molecular structure
(of bisphosphinoferrocene metal complexes)
IT Fluxional rearrangement
(of chromium or molybdenum bisphosphinoferrocene complexes)
IT 95408-44-9
RL: PRP (Properties)
(crystal structure of)
IT 67292-28-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluxionality and mol. structure of)
IT 67292-31-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluxionality of)
IT 83547-83-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with chlorophosphines)
IT 72954-06-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reactions of, with chlorophosphine)
IT 67292-33-5P 95464-05-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT 72287-26-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

IT 95408-39-2P 95408-40-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, with metal complex)

IT 95408-38-1P 95464-04-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reactions of, with metal complexes)

IT 12098-17-8P **92269-95-9P 92284-07-6P** 95408-41-6P
 95408-42-7P 95408-45-0P 95408-46-1P 95408-47-2P 95408-48-3P
 95408-49-4P 95408-51-8P 95408-52-9P 95420-22-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 1079-66-9 13716-10-4 29949-69-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, for lithiated phosphinoferrocene)

IT 10025-98-6 12107-56-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with bisphosphinoferrocene complexes)

IT 95408-37-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chlorophosphine)

IT 12150-46-8 84680-95-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with palladium or nickel complex)

IT 14220-64-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactions of, with bisphosphinoferrocene complexes)

IT **92269-95-9P 92284-07-6P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 92269-95-9 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-
 dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate
 (9CI) (CA INDEX NAME)

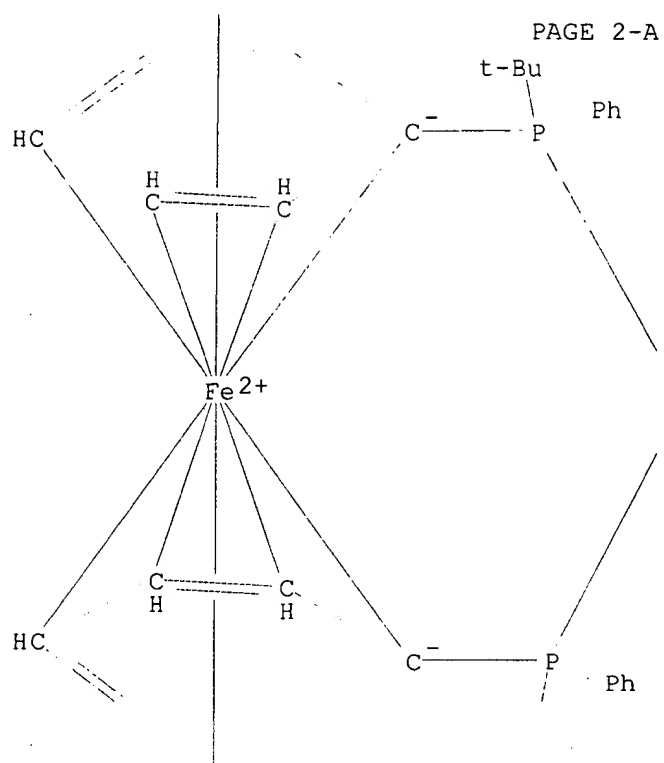
CM 1

CRN 92269-94-8

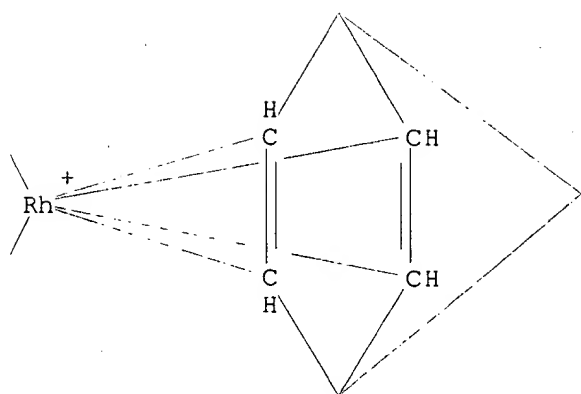
CMF C37 H44 Fe P2 Rh

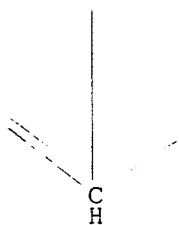
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



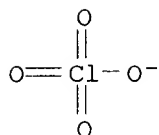


PAGE 3-A
t-Bu

CM 2

CRN 14797-73-0

CMF C1 O4



RN 92284-07-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

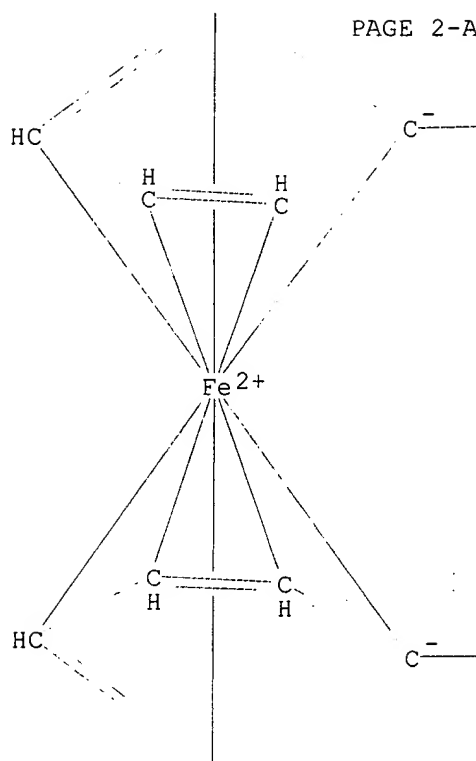
CRN 92284-06-5

CMF C37 H44 Fe P2 Rh

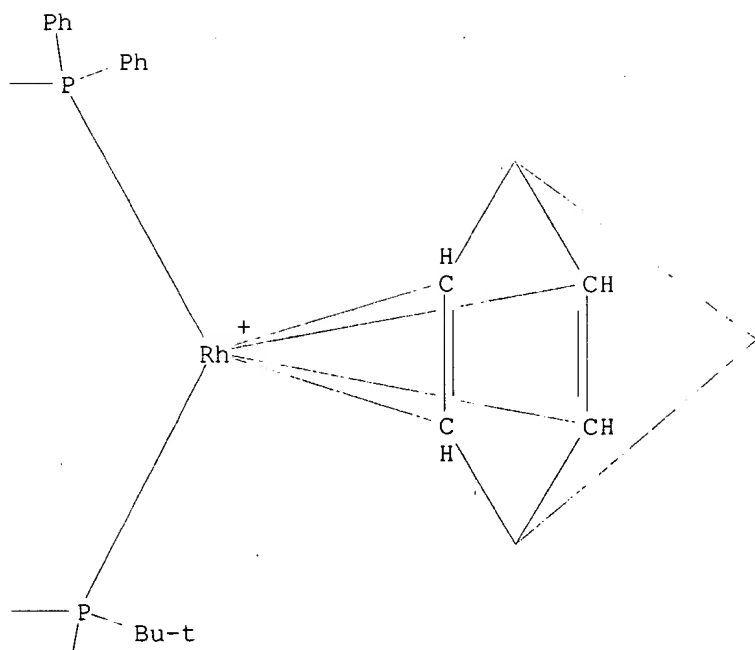
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
H

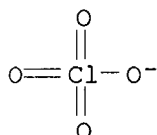
PAGE 3-B

t-Bu

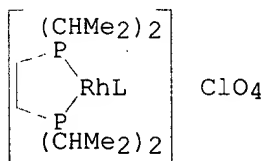
CM 2

CRN 14797-73-0

CMF C1 04



L104 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1985:185249 HCAPLUS
 DN 102:185249
 ED Entered STN: 02 Jun 1985
 TI **Hydrogenation** of cationic bis(tertiary alkylphosphine)
rhodium(I) complexes. An NMR study
 AU Butler, Ian R.; Cullen, William R.; Mann, Brian E.; Nurse, Charles R.
 CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
 SO Journal of Organometallic Chemistry (1985), 280(2), C47-C50
 CODEN: JORCAI; ISSN: 0022-328X
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 GI



I

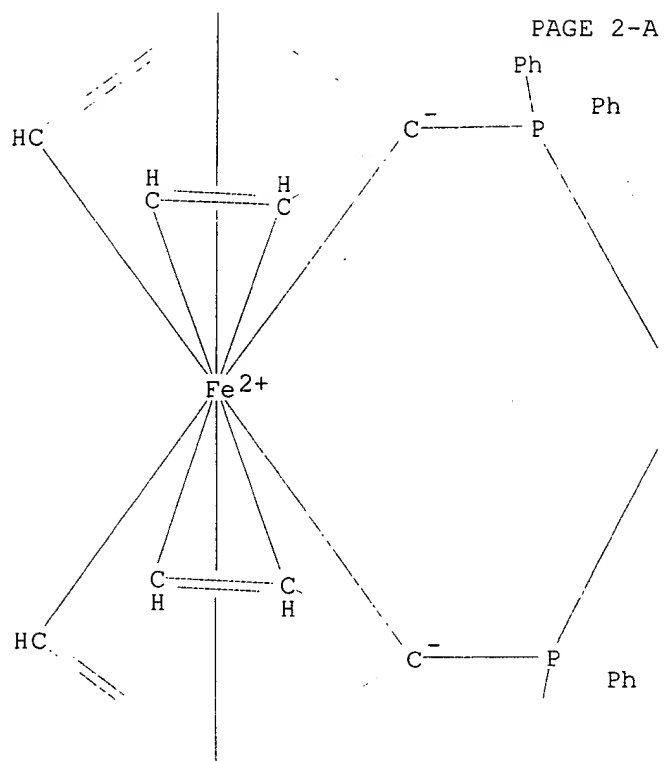
AB **Rhodium** hydrides have been observed in solution in the reaction of
 cationic **rhodium(I)** complexes of bis(tertiary phosphines), e.g.,
 (I, L = norbornadiene) with H.
 ST **hydrogenation phosphinerhodium** complex;

rhodium phosphine hydrogenation; hydride rhodium
phosphine; NMR hydrogenation phosphinerhodium complex
IT Nuclear magnetic resonance
(of hydrogenation of rhodium phosphine complexes)
IT Hydrogenation
(of rhodium phosphine complexes)
IT 84680-96-6 92269-95-9 96144-39-7 96144-63-7
96144-65-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
IT 96144-41-1P 96144-67-1P 96144-69-3P
96144-71-7P 96144-73-9P 96144-75-1P
96144-77-3DP, perchlorate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 84680-96-6 92269-95-9 96144-63-7
96144-65-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
RN 84680-96-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX
NAME)

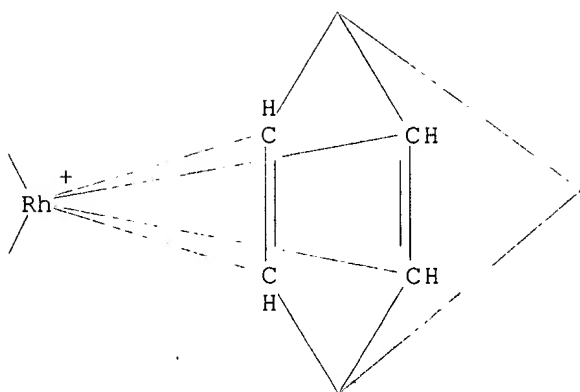
CM 1

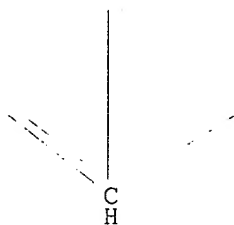
CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B





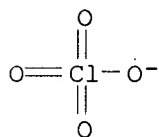
PAGE 3-A

Ph

CM 2

CRN 14797-73-0

CMF C1 O4



RN 92269-95-9 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

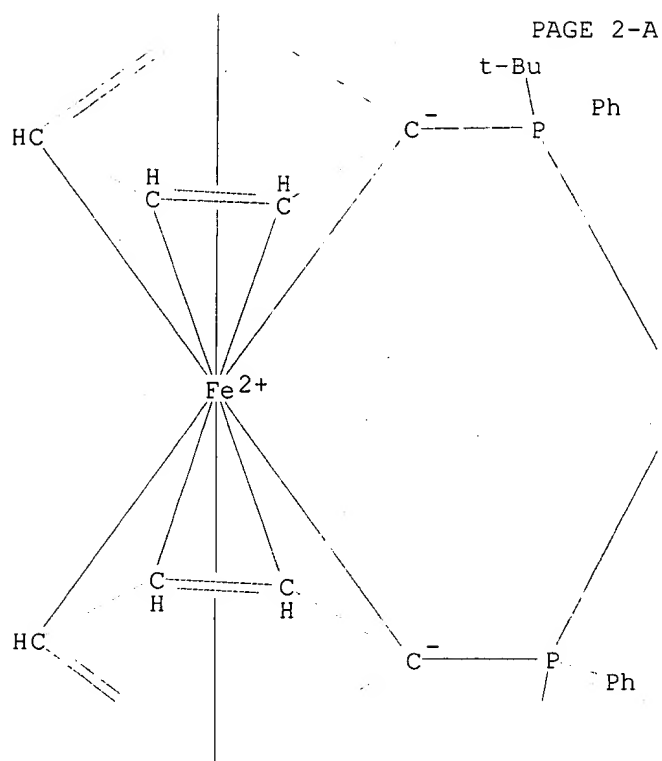
CM 1

CRN 92269-94-8

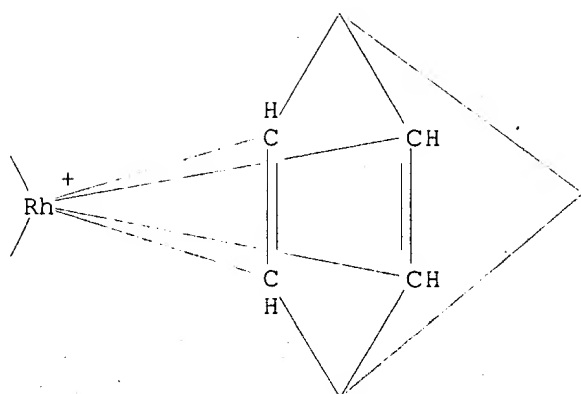
CMF C37 H44 Fe P2 Rh

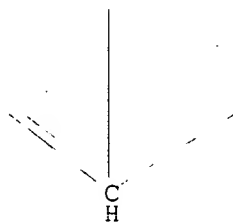
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B

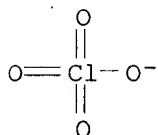




PAGE 3-A
t-Bu

CM 2

CRN 14797-73-0
CMF C1 O4



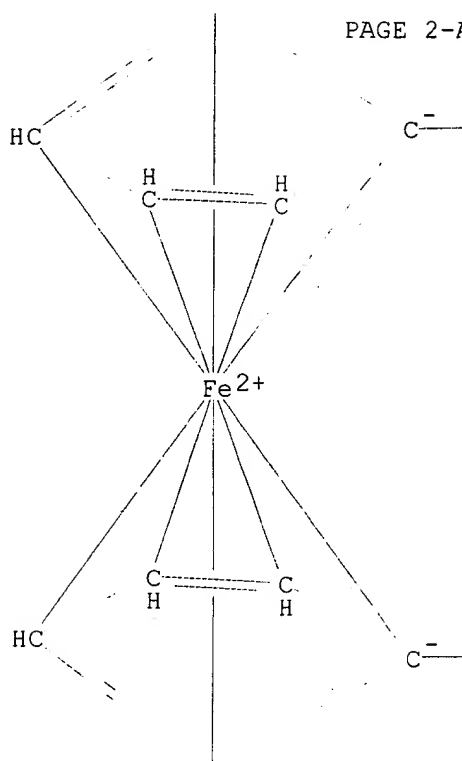
RN 96144-63-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

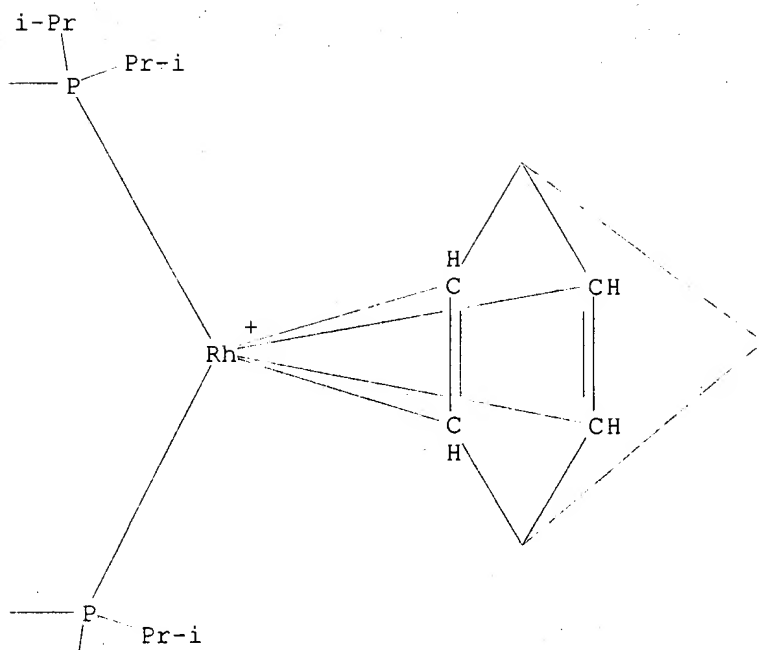
CRN 96144-62-6
CMF C29 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
H

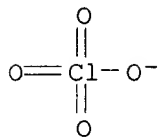
PAGE 3-B

i-Pr

CM 2

CRN 14797-73-0

CMF C1 O4



RN 96144-65-9 ' HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1-methylethyl)phenylphosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

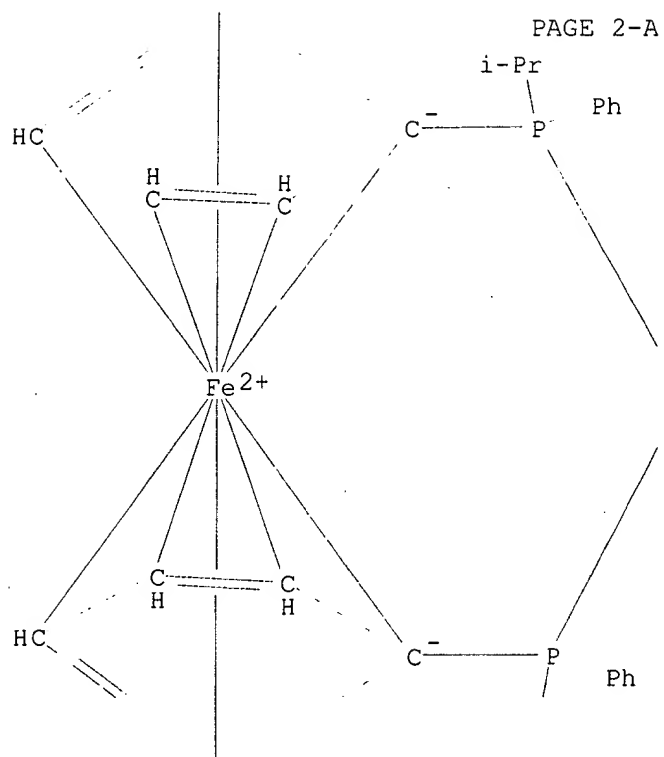
CM 1

CRN 96144-64-8

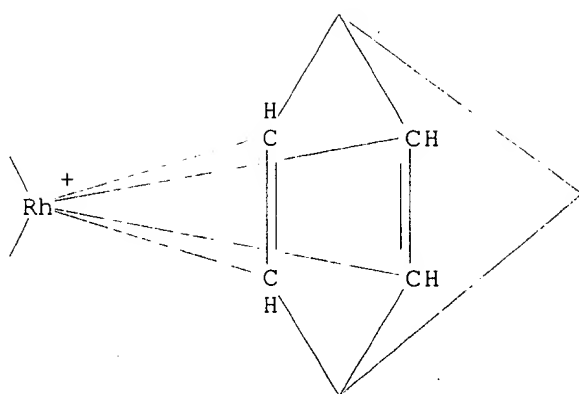
CMF C35 H40 Fe P2 Rh

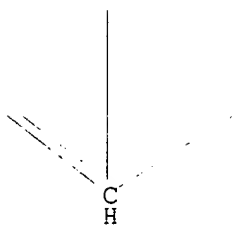
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



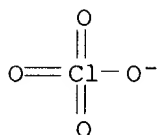


PAGE 3-A
i-Pr

CM 2

CRN 14797-73-0

CMF Cl O4



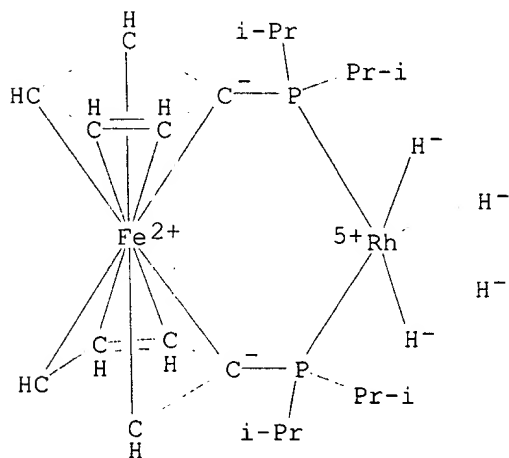
IT 96144-67-1P 96144-69-3P 96144-71-7P
96144-73-9P 96144-75-1P 96144-77-3DP,
perchlorate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 96144-67-1 HCAPLUS
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-
P,P']tetrahydro-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-66-0

CMF C22 H40 Fe P2 Rh

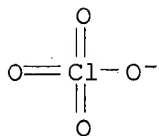
CCI CCS



CM 2

CRN 14797-73-0

CMF C1 O4



RN 96144-69-3 HCAPLUS

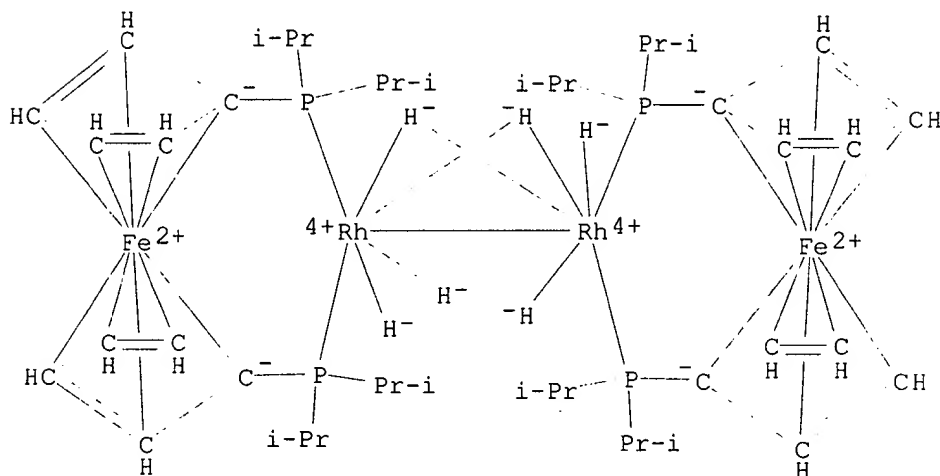
CN Rhodium(2+), bis[1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']di- μ -hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-68-2

CMF C44 H78 Fe2 P4 Rh2

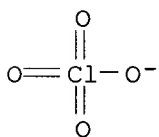
CCI CCS



CM 2

CRN 14797-73-0

CMF C1 O4



RN 96144-71-7 HCAPLUS

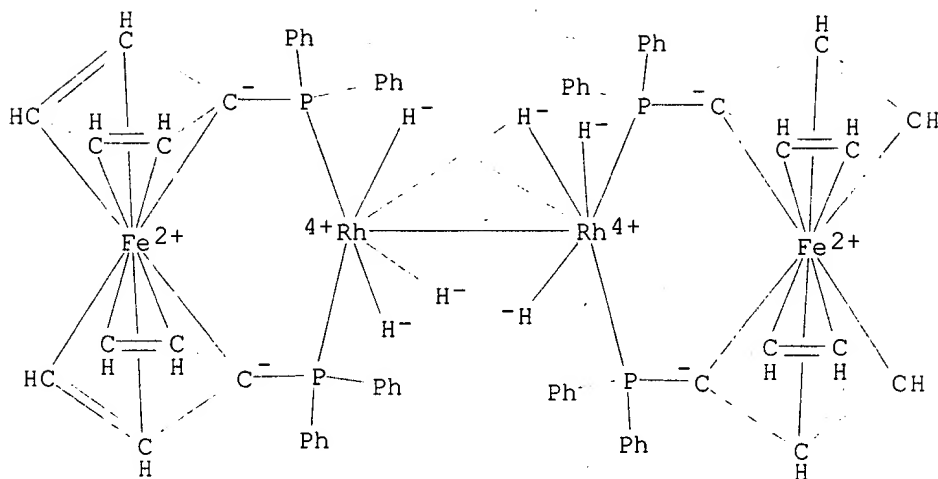
CN Rhodium(2+), bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di- μ -hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-70-6

CMF C68 H62 Fe2 P4 Rh2

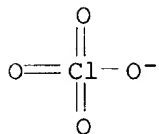
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 96144-73-9 HCAPLUS

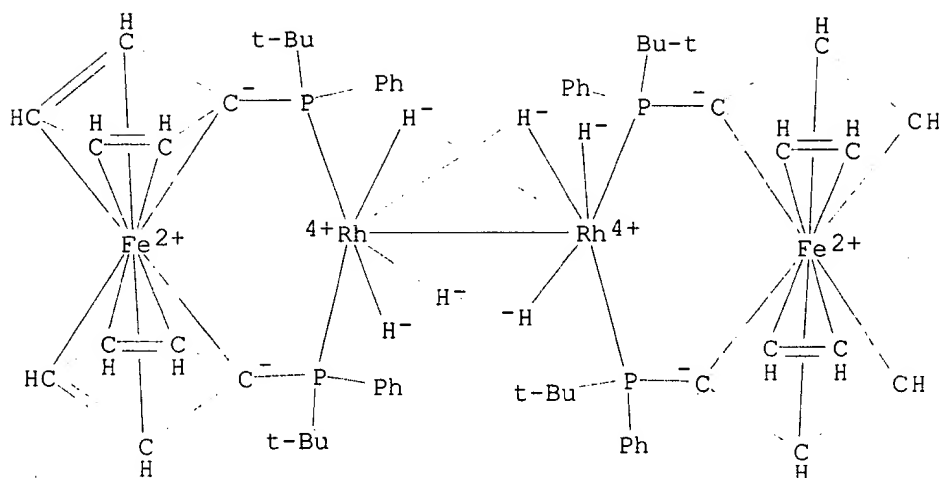
CN Rhodium(2+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']di-μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-72-8

CMF C60 H78 Fe2 P4 Rh2

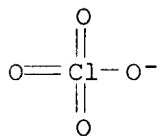
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 96144-75-1 HCAPLUS

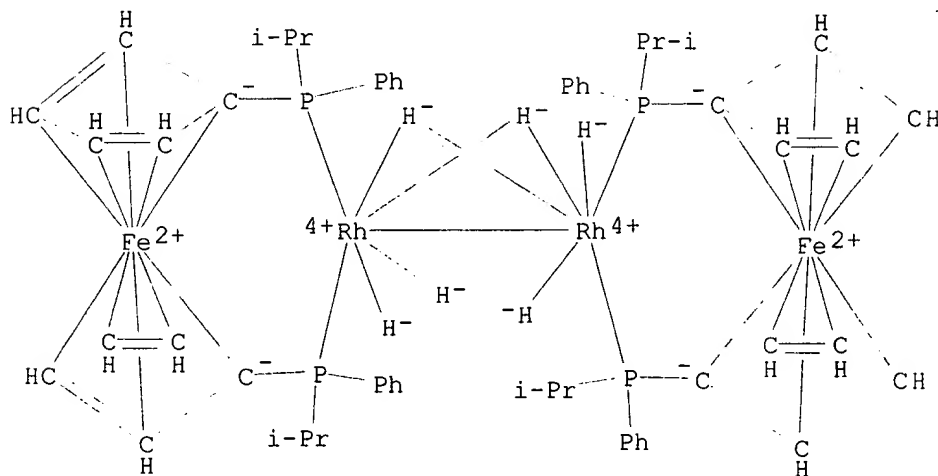
CN Rhodium(2+), bis[1,1'-bis[(1-methylethyl)phenylphosphino]ferrocene-P,P']di-
μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-74-0

CMF C56 H70 Fe2 P4 Rh2

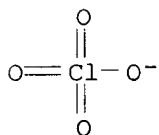
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CM 2

CRN 14797-73-0

CMF Cl O4



RN 96144-77-3 HCAPLUS

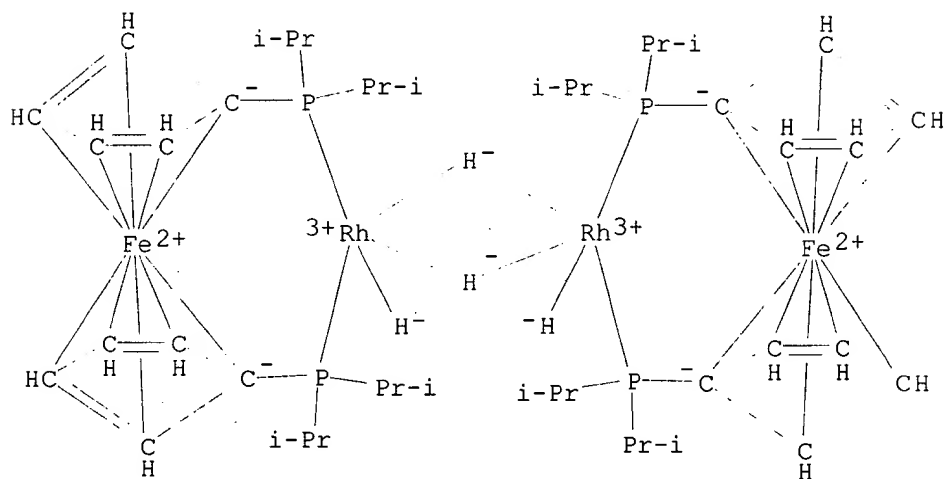
CN Rhodium(2+), bis[1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']di-
μ-hydrodihydrodi-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-76-2

CMF C44 H76 Fe2 P4 Rh2

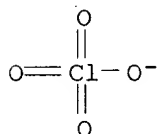
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



L104 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:166925 HCAPLUS

DN 102:166925

ED Entered STN: 18 May 1985

TI **Rhodium**(I) complexes of ferrocenylphosphines as efficient asymmetric catalysts. The structure of $\text{Fe}(\eta^5\text{-C}_5\text{H}_3(\text{P}(\text{CMe}_3)_2\text{-1,3})(\eta^5\text{-C}_5\text{H}_3(\text{CHMeNMe}_2)\text{P}(\text{CMe}_3)_2\text{-1,2}))$

AU Appleton, Trevor D.; Cullen, William R.; Evans, Stephen V.; Kim, Tae Jeong; Trotter, James

CS Dep. Chem., Univ. Br. Columbia, Vancouver, BC, V6T 1Y6, Can.

SO Journal of Organometallic Chemistry (1985), 279(1-2), 5-21
CODEN: JORCAI; ISSN: 0022-328X

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 25, 67, 75

OS CASREACT 102:166925

GI For diagram(s), see printed CA Issue.

AB The chiral aminomethylferrocenes (R)- or (S)-I (R-R2 = H) were lithiated and treated with $\text{ClP}(\text{CMe}_3)_2$ under varying reaction conditions to give (R,S)-I [R = $\text{P}(\text{CMe}_3)_2$; R1 = H (II), $\text{P}(\text{CMe}_3)_2$ (III); R2 = H] and (S,R)-I (same R's) resp. Similarly, (R, R)- or (S, S)-I [R = R2 = $\text{P}(\text{CMe}_3)_2$, R1 = H] (IV) were prepared from (R)- or (S)-I (R-R2 = H) resp. [Rh(NBD)L]ClO4 [V; NBD = norbornadiene, L = (S,R)-II, (S,R)-III, (S,S)-IV] catalyzed asym **hydrogenation** of $\text{H}_2\text{C:CR}_3\text{CO}_2\text{H}$ (R3 = Me, $\text{CH}_2\text{CO}_2\text{H}$) and $\text{PhCH:CR}_4\text{CO}_2\text{H}$ (R4 = NHAc, Me); V [L = (S,S)-IV] gave products with up to 95% enantiomeric excesses. The x-ray crystal structure of (S,S)-IV showed the cyclopentadienyl rings are close to planar, deviate slightly from coplanarity, and are rotated by about 7° from an eclipsed conformation. The substituent P and C atoms are significantly displaced from the ring planes.

ST crystal structure ferrocenyltriposphine chiral; mol structure ferrocenyltriposphine chiral; ferrocenylphosphine structure **rhodium** complex catalyst; **rhodium** ferrocenylphosphine complex **hydrogenation** asym

IT Crystal structure
Molecular structure
(of ferrocenyltriposphine complex, chiral)

IT Asymmetric synthesis and induction
(of organic acids, by **hydrogenation** of olefinic acids, **rhodium**-ferrocenylphosphine catalyst for)

IT **Hydrogenation**
(asym., of olefinic acids)

IT **Hydrogenation catalysts**
(asym., **rhodium**-ferrocenyltriphenylphosphine complex, for olefinic acids)

IT 97-65-4, reactions 1895-97-2 5429-56-1 55065-02-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. **hydrogenation** of, **rhodium**-ferrocenylphosphine complex for)

IT 95840-92-9
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for asym. **hydrogenation** of olefinic acids)

IT 83356-93-8 95839-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with **rhodium** complex)

IT 31886-57-4 31886-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and phosphination of)

IT 95762-74-6P 95839-79-5P 95840-91-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium**)

IT 95839-76-2P 95839-78-4P 95840-90-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of)

IT 97-69-8P 2018-61-3P 2174-58-5P 3641-51-8P 10172-89-1P

14367-54-5P 14367-67-0P 19436-52-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by asym. **hydrogenation** of olefinic acid,
rhodium-ferrocenyltriposphine complex for)

IT 95762-71-3P 95762-73-5P 95840-45-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, conformation, and catalyst activity of, for asym.
hydrogenation)

IT 95762-75-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, crystal structure, and complexation of, with **rhodium**
)

IT 13716-10-4

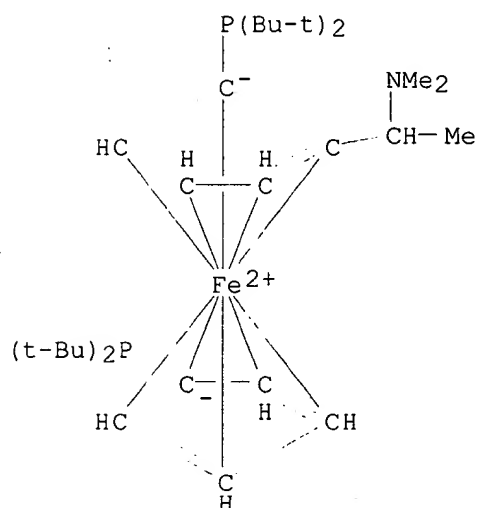
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chiral aminoferrocene)

IT 95762-74-6P 95839-79-5P 95840-91-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation of, with **rhodium**)

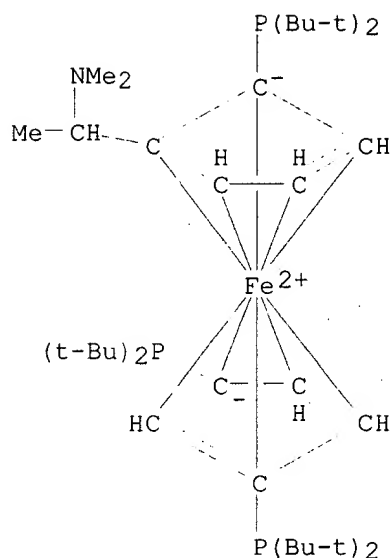
RN 95762-74-6 HCAPLUS

CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)



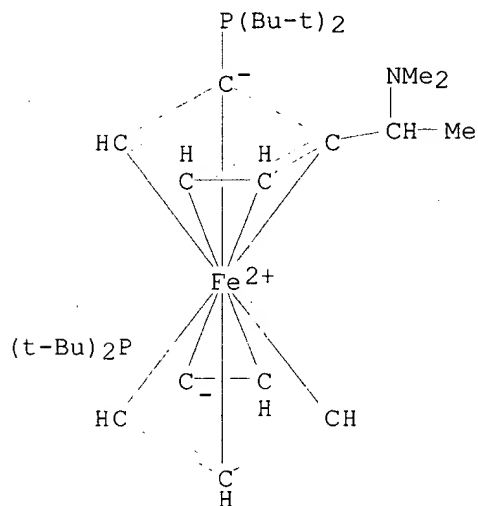
RN 95839-79-5 HCAPLUS

CN Ferrocene, 1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)



RN 95840-91-8 HCAPLUS

CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



IT 95839-76-2P 95839-78-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of)

RN 95839-76-2 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, [R-(R*,R*)]-, perchlorate. (9CI) (CA INDEX NAME)

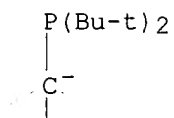
CM 1

CRN 95839-75-1

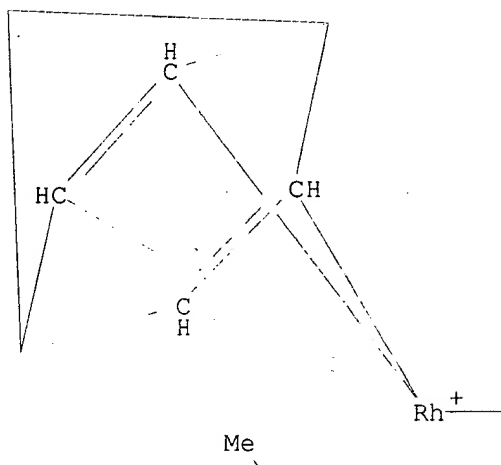
CMF C37 H61 Fe N P2 Rh

CCI CCS

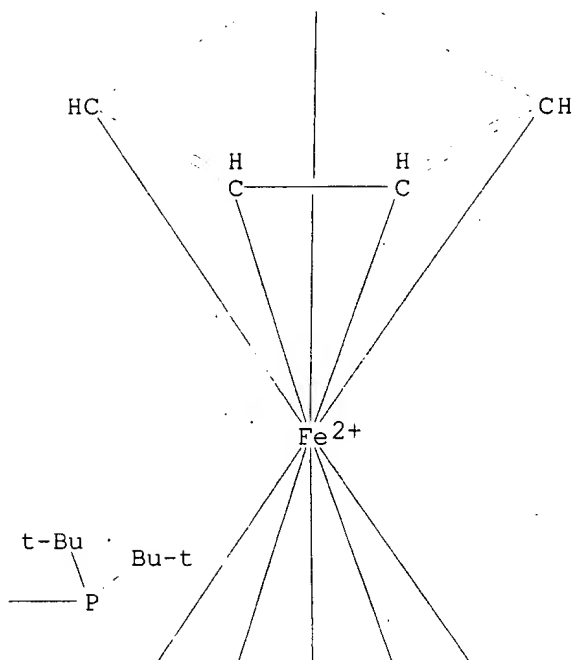
PAGE 1-B



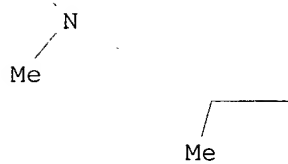
PAGE 2-A



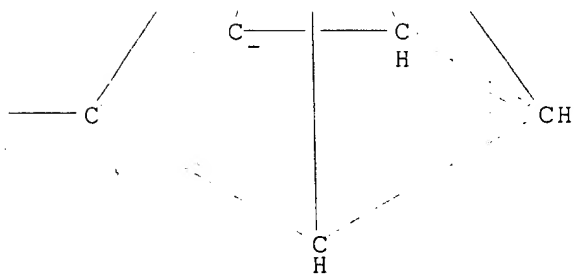
PAGE 2-B



PAGE 3-A



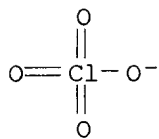
PAGE 3-B



CM 2

CRN 14797-73-0

CMF C1 04

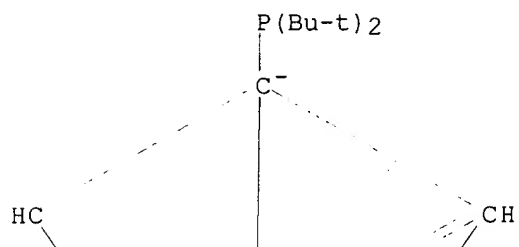


RN 95839-78-4 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, [S-(R*,S*)]-, perchlorate (9CI) (CA INDEX NAME)

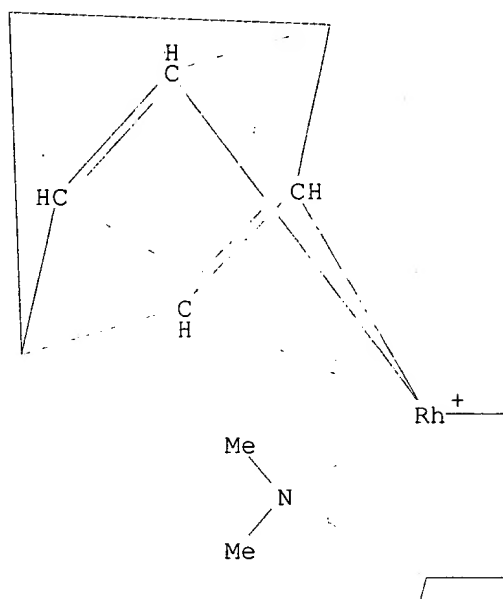
CM 1

CRN 95839-77-3
 CMF C45 H78 Fe N P3 Rh
 CCI CCS

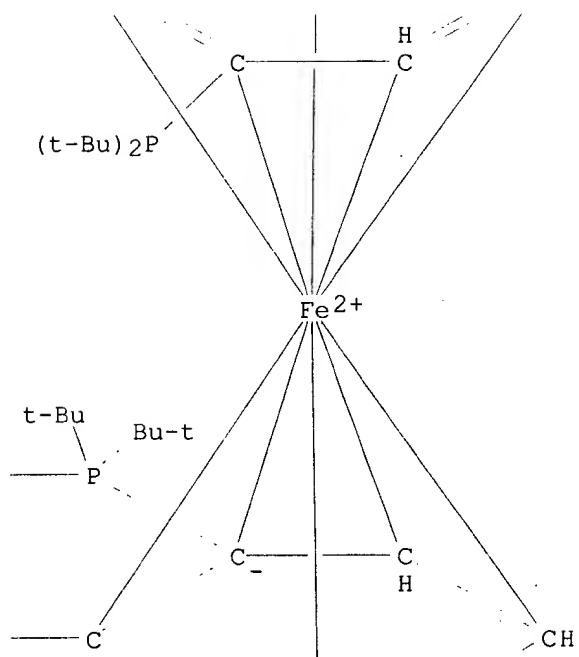
PAGE 1-B



PAGE 2-A



PAGE 2-B



PAGE 3-A
Me

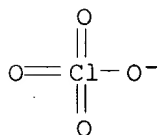
PAGE 3-B



CM 2

CRN 14797-73-0

CMF C1 O4



IT 95762-71-3P 95762-73-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation, conformation, and catalyst activity of, for asym.

hydrogenation)

RN 95762-71-3 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

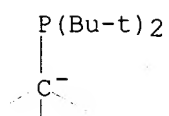
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CRN 95762-70-2

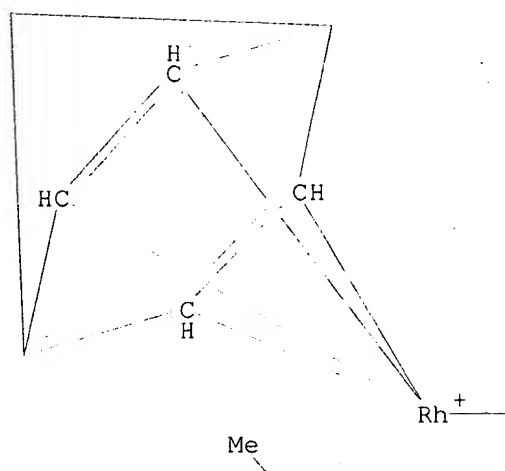
CMF C37 H61 Fe N P2 Rh

CCI CCS

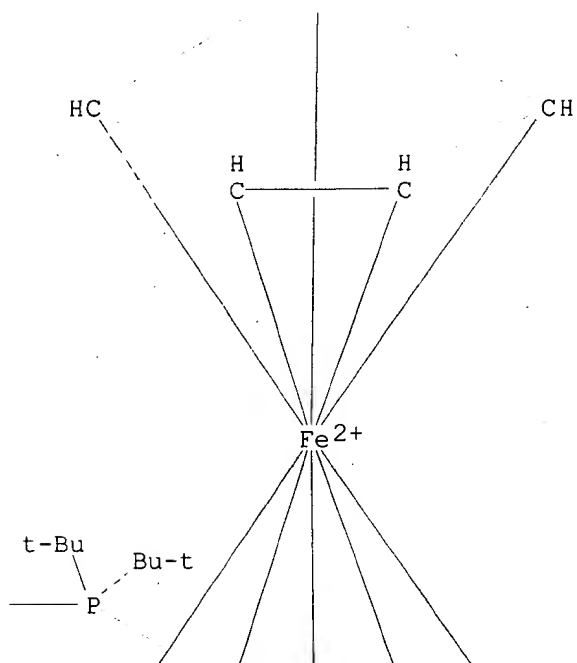
PAGE 1-B



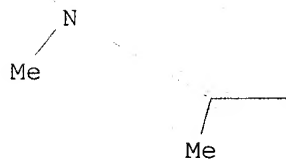
PAGE 2-A



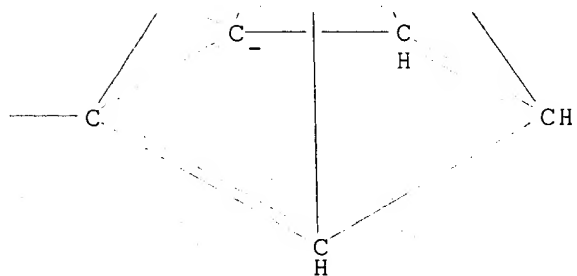
PAGE 2-B



PAGE 3-A



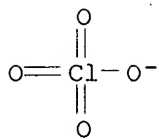
PAGE 3-B



CM 2

CRN 14797-73-0

CMF C1 04



RN 95762-73-5 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1',3-tris[bis(1,1-dimethylethyl)phosphino]-2'-[1-(dimethylamino)ethyl]ferrocene-N2',P1']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

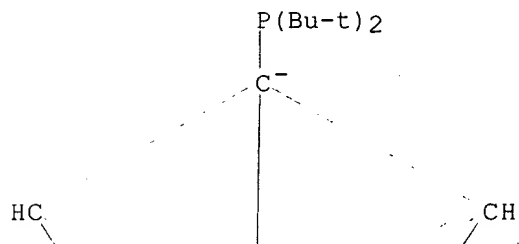
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CRN 95762-72-4

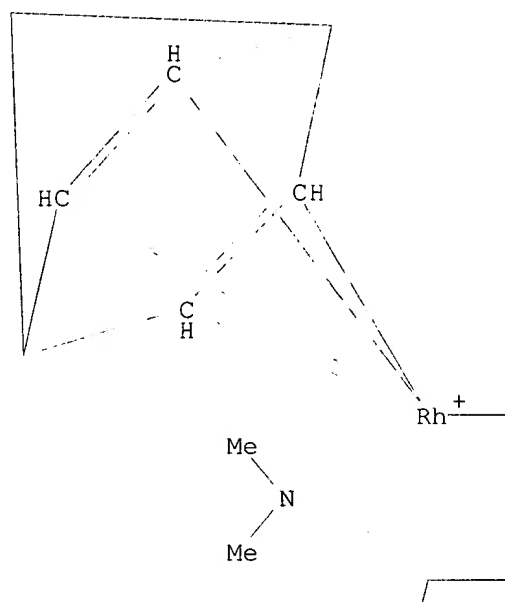
CMF C45 H78 Fe N P3 Rh

CCI CCS

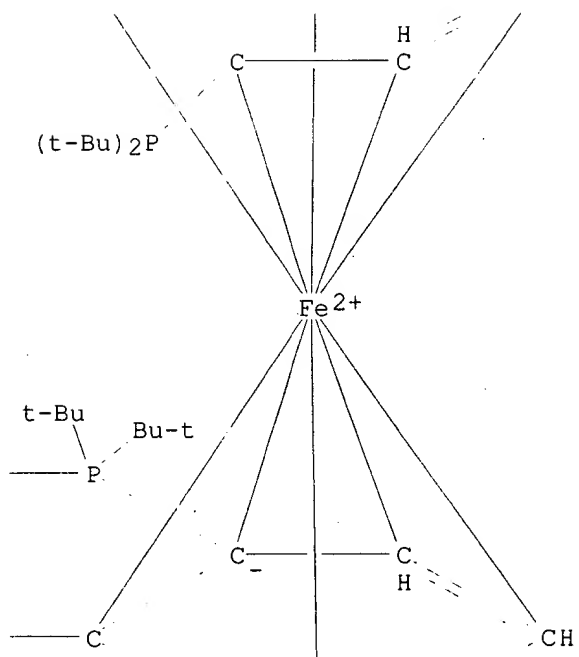
PAGE 1-B



PAGE 2-A



PAGE 2-B



PAGE 3-A

Me

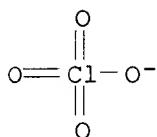
PAGE 3-B



CM 2

CRN 14797-73-0

CMF C1 04

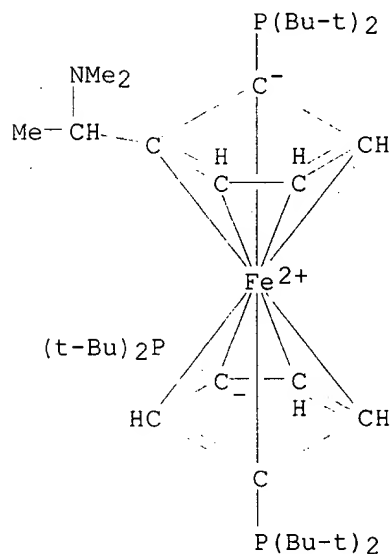


IT 95762-75-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and complexation of, with rhodium)

RN 95762-75-7 HCAPLUS

CN Ferrocene, 1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)



L104 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:158448 HCAPLUS

DN 102:158448

ED Entered STN: 04 May 1985

TI Crystallographic analysis of two rhodium(III) hydride complexes,
bis{1,1'-bis[tert-butyl(phenyl)phosphino]ferrocene-P,P'}-tri-μ-hydrido-

dihydridodirrhodium(III) chlorate methanol solvate,
 [Rh₂H₅{Fe[P(C₄H₉)(C₅H₄)(C₆H₅)]₂}]₂]ClO₄.CH₃OH (I), and bis[1,1'-bis(di-tert-butylphosphino)ferrocene-P,P']-tri-μ-hydrido-dihydridodirrhodium(III) chlorate, [Rh₂H₅{Fe[P(C₄H₉)₂(C₅H₄)]₂}]₂]ClO₄ (II)

AU Einstein, F. W. B.; Jones, T.
 CS Dep. Chem., Simon Fraser Univ., Burnaby, BC, V5A 1S6, Can.
 SO Acta Crystallographica, Section C: Crystal Structure Communications (1985), C41(3), 365-9
 CODEN: ACSCEE; ISSN: 0108-2701

DT Journal
 LA English
 CC 75-8 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 29, 78

AB Title compound (I) is monoclinic, space group P2₁/n, with a 18.708(4), b 14.857(2), c 21.853(4) Å, and β 92.95(2)°; Z = 4 for d = 1.501. The final R = 0.045 for 5732 reflections. Title compound (II) is monoclinic, space group P2₁/c, with a 15.276(3), b 14.751(2), c 25.950(3) Å, and β 90.85(1)°; Z = 4, for d = 1.430. The final R = 0.059 for 4180 reflections. The structure of I contains an unusual RhPH skeletal structure in which each Rh atom (in the 3+ oxidation state) has 3 Rh-H bridging bonds [average 1.77(8) Å], a single Rh-H terminal bond [average 1.56(12) Å] and 2 Rh-P bonds. It is tentatively proposed that II contains a similar arrangement. Atomic coordinates are given.

ST mol structure rhodium hydro bridged phosphinoferrocene; ferrocene butylphosphino rhodium hydro structure

IT Crystal structure
 Molecular structure
 (of rhodium hydro-bridged butylphenylphosphinoferrocene and dibutylphosphinoferrocene complexes)

IT 92468-68-3 95783-24-7
 RL: PRP (Properties)
 (structure of)

IT 92468-68-3
 RL: PRP (Properties)
 (structure of)

RN 92468-68-3 HCAPLUS
 CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, stereoisomer, perchlorate, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1
 CMF C H4 O

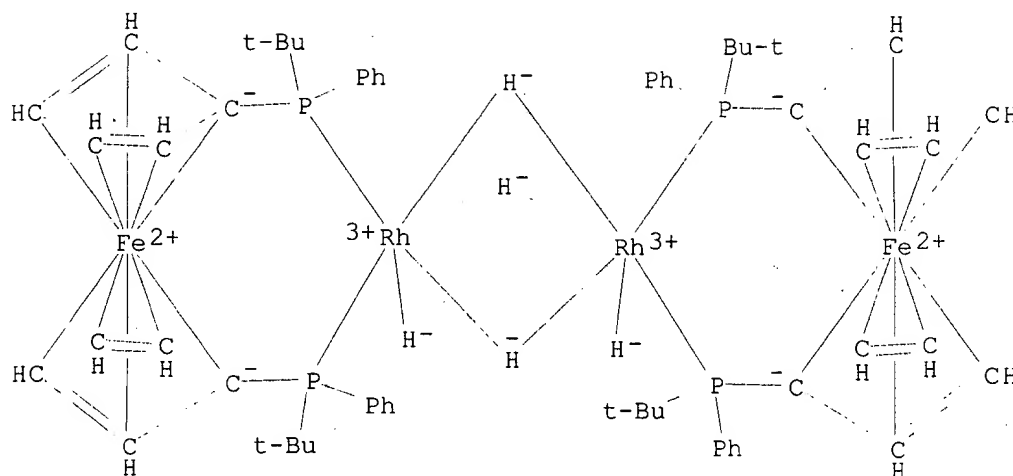
H₃C-OH

CM 2

CRN 92468-67-2
 CMF C60 H77 Fe2 P4 Rh2 . Cl O4

CM 3

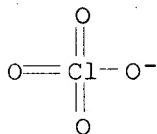
CRN 92468-66-1
 CMF C60 H77 Fe2 P4 Rh2
 CCI CCS



CM 4

CRN 14797-73-0

CMF Cl O4



L104 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:79103 HCAPLUS

DN 102:79103

ED Entered STN: 09 Mar 1985

TI Structures of three **hydrogenation** catalysts [(P-P)Rh
(NBD)]ClO4 and some comparative rate studies where (P-P) =
(η5-R1R2PC5H4)(η5-R3R4PC5H4)Fe (R1 = R2 = R3 = R4 = Ph; R1 = R2 =
Ph, R3 = R4 = CMe3; R1 = R3 = Ph, R2 = R4 = CMe3)

AU Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones,
Terry

CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SO Organometallics (1985), 4(2), 346-51

CODEN: ORGND7; ISSN: 0276-7333

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

AB Bulky Me3C groups enhance the **hydrogenation** rates of alkenes
(except for bulky substrates) at 30°/1 atm H2 using the title
compds. [(P-P)RhNBD]ClO4 [(P-P) = (η5-R1R2PC5H4)Fe(η5-R3R4PC5H4);
R1 = R2 = R3 = R4 = Me3C (I), Ph (II); R1 = R2 = Me3C, R3 = R4 = Ph (III);
R1 = R3 = Me3C, R2 = R4 = Ph (IV)] as catalyst precursors. The most
promising combination of steric and electronic effects exists with
(±)-IV. Crystallog. of II, III, and IV show that the bulky Me3C groups
cause a lengthening of P-Rh distances, wider P-Rh-P
angles, and a rotation of the norbornadiene group out of the P-Rh
-P plane. Generally the effects range from a maximum in I (previously
determined)

to a min. in II.

ST crystal structure **rhodium** phosphine complex; mol structure **rhodium** phosphine complex; steric effect **hydrogenation** catalyst; ferrocenebisphosphine **rhodium** complex butyl group

IT tert-Butyl group
(effect of, on **hydrogenation** of alkenes using ferrocenebis(phosphine)**rhodium** complex catalyst)

IT **Hydrogenation catalysts**
(ferrocenebis(phosphine) **rhodium** complexes, for alkenes, kinetics and mechanism with)

IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, **rhodium** phosphine catalyst for)

IT Bond angle
Bond length
(in ferrocenebis(phosphine) **rhodium** complexes)

IT Kinetics of **hydrogenation**
(of alkenes in presence of ferrocenebis(phosphine) **rhodium** complexes)

IT **Hydrogenation**
(of alkenes in presence of ferrocenebis(phosphine) **rhodium** complexes, mechanism of)

IT Crystal structure
Molecular structure
(of ferrocenebis(phosphine) **rhodium** complexes)

IT Substituent effect
(on catalytic activity of ferrocene bis(phosphine)**rhodium** complex in **hydrogenation** of alkenes)

IT Steric effect
(on **hydrogenation** of alkenes using ferrocenebis(phosphine) **rhodium** complexes)

IT 84680-96-6 92269-95-9 92284-07-6
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, crystallog. in relation to kinetics and mechanism with)

IT 84680-98-8
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, mol. structure in relation to kinetics and mechanism with)

IT 97-65-4, reactions 110-83-8, reactions 1199-77-5 5429-56-1 5469-45-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, using ferrocenebis(phosphine) **rhodium** complexes, kinetics and mechanism of)

IT 84680-96-6 92269-95-9 92284-07-6
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, crystallog. in relation to kinetics and mechanism with)

RN 84680-96-6 HCAPLUS

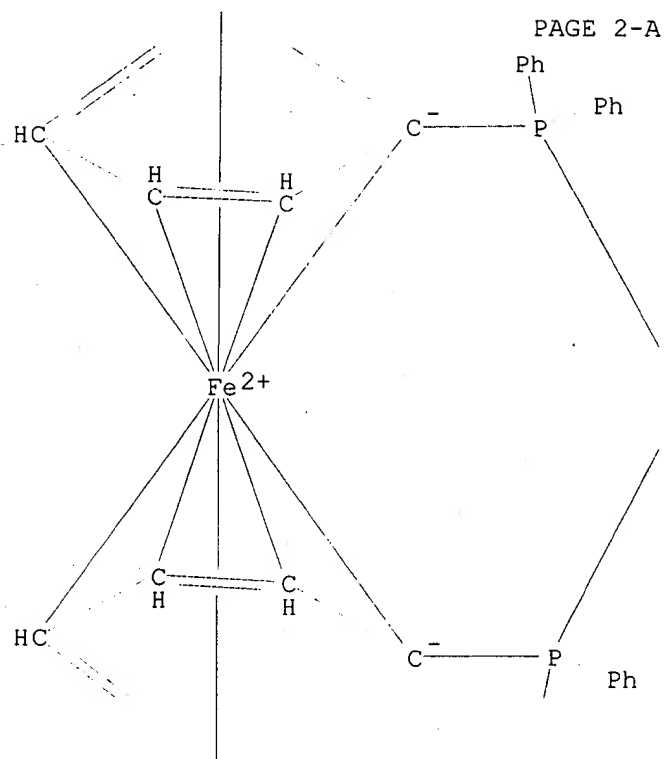
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

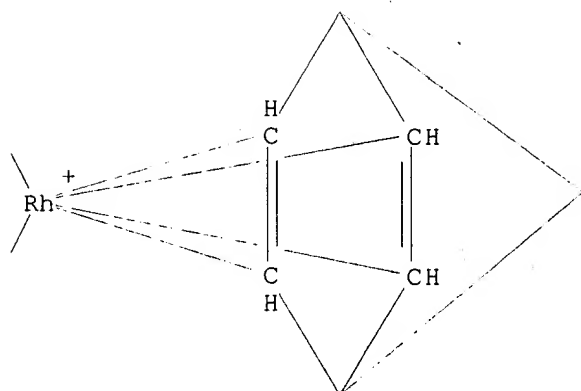
CRN 79790-97-9

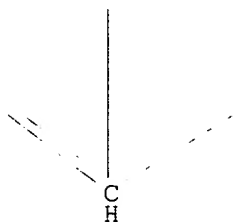
CMF C41 H36 Fe P2 Rh

CCI CCS



PAGE 2-B





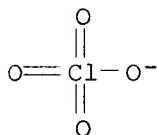
PAGE 3-A

Ph

CM 2

CRN 14797-73-0

CMF C1 O4



RN 92269-95-9 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

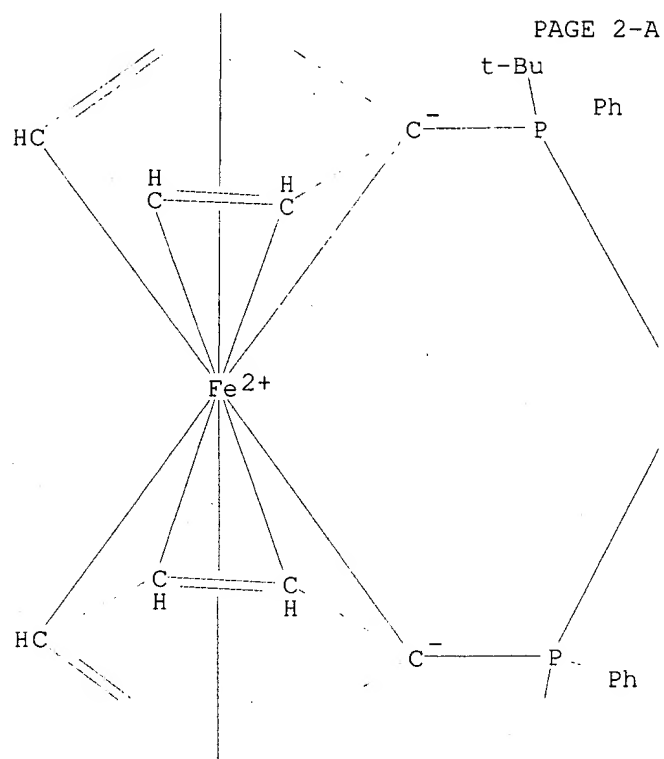
CM 1

CRN 92269-94-8

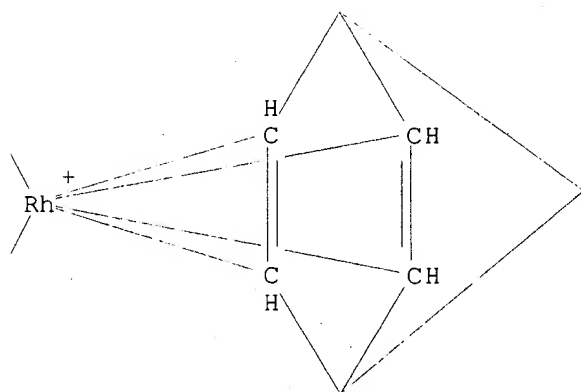
CMF C37 H44 Fe P2 Rh

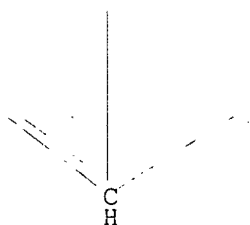
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



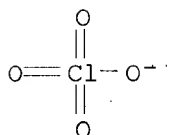


PAGE 3-A
t-Bu

CM 2

CRN 14797-73-0

CMF C1 O4



RN 92284-07-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene] [1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

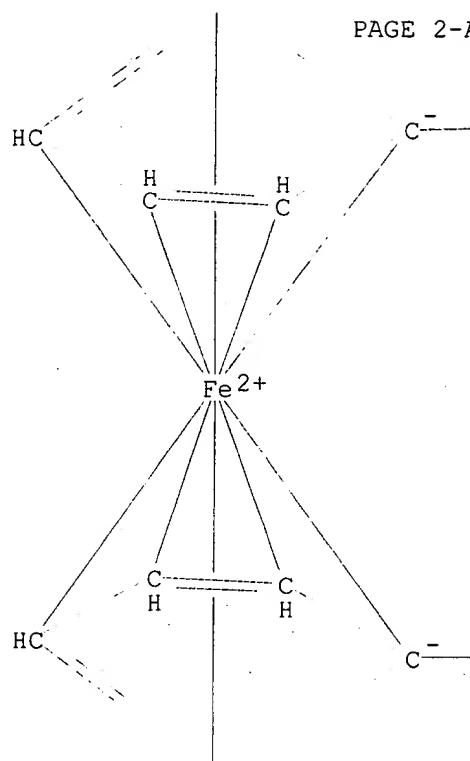
CRN 92284-06-5

CMF C37 H44 Fe P2 Rh

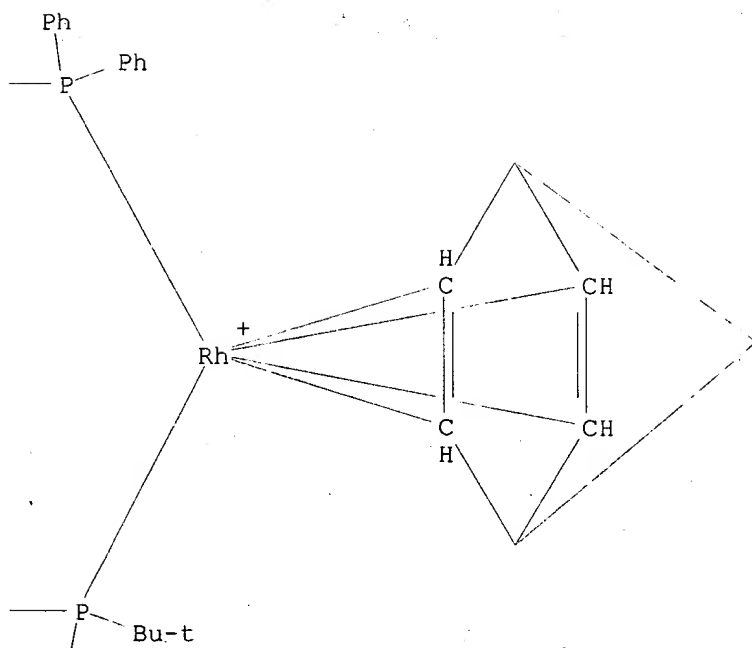
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
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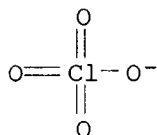
PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0

CMF C1 O4



IT 84680-98-8

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for **hydrogenation** of alkenes, mol. structure in relation to kinetics and mechanism with)

RN 84680-98-8 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI)
(CA INDEX NAME)

CM 1

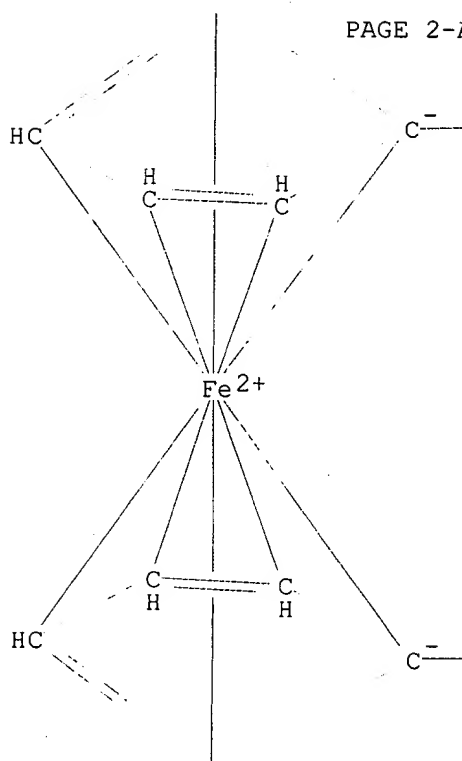
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CMF C33 H52 Fe P2 Rh

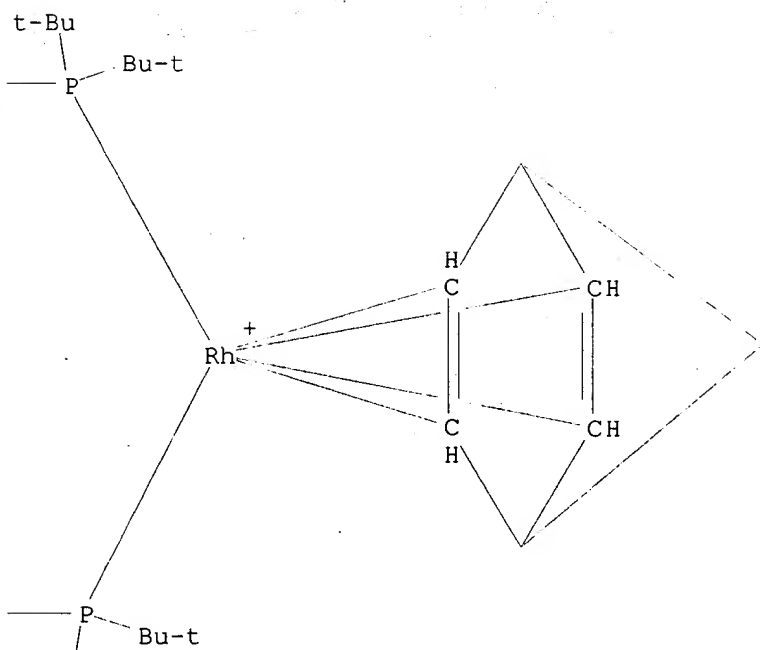
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A



C
H

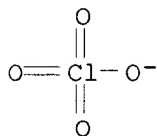
PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0

CMF Cl O4



L104 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1984:571461 HCAPLUS

DN 101:171461

ED Entered STN: 10 Nov 1984

TI Metal hydrides from cationic **rhodium**(I) catalyst precursors.X-ray structure of [(L-L)HRh(μ -H)3Rh(L-L)]ClO4 [L-L =
rac-Fe(η 5-C5H4PPhCMe3)2]AU Butler, Ian R.; Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W.
B.; Jones, Terry

CS Chem. Dep.; Univ. British Columbia, Vancouver, V6T 1Y6, Can.

SO Journal of the Chemical Society, Chemical Communications (1984),
(11), 719-21

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 67, 75

AB Treatment of [LRhL1]ClO4 [L = rac-Fe(η 5-C5H4PPhCMe3)2,
Fe(η 5-C5H4P(CMe3)2)2 (C5H5 = cyclopentadienyl), L1 = norbornadiene]
with H in MeOH at 30° and 1 atm gave [LHRh(μ -H)3RhLH]ClO4 (L as
before) (II and III, resp.). The structures of II and III were determined by
x-ray anal.ST **rhodium** ferrocenylphosphine hydride crystal structure; catalyst
rhodium ferrocenylphosphine **hydrogenation**

IT Crystal structure

Molecular structure

(of hydride-bridged **rhodium** ferrocenylphosphines)

IT 84680-98-8 92269-95-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of)

IT 92468-68-3P 92468-70-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal and mol. structure of)

IT 92468-67-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mol. structure of)

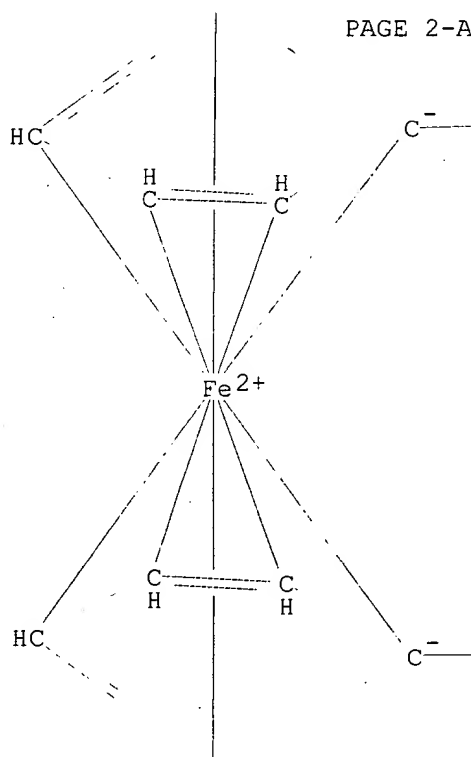
IT 84680-98-8 92269-95-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of)

RN 84680-98-8 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
 bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI)
 (CA INDEX NAME)

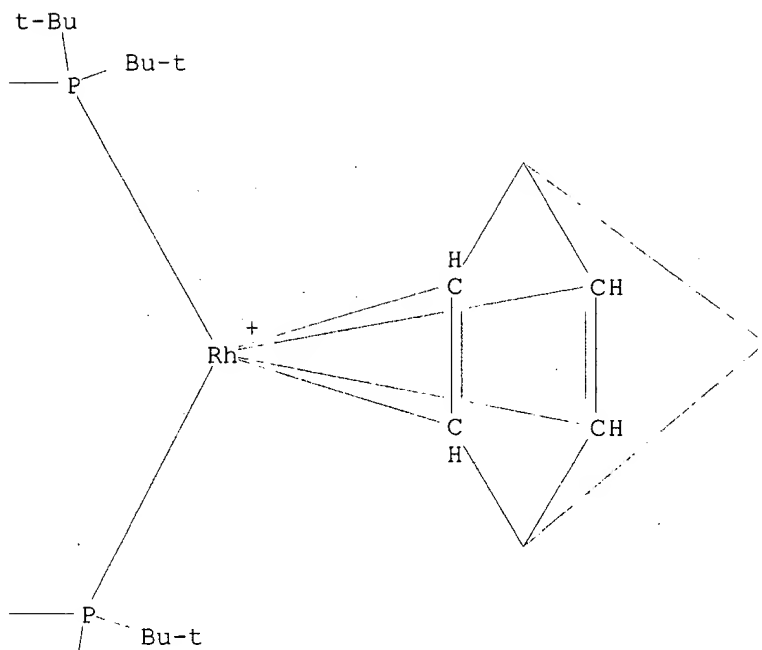
CM 1

CRN 84680-97-7
 CMF C33 H52 Fe P2 Rh
 CCI CCS

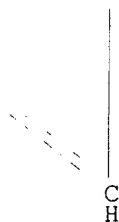
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B



PAGE 3-A



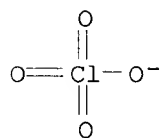
PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0

CMF C1 O4



RN 92269-95-9 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-

dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate
(9CI) (CA INDEX NAME)

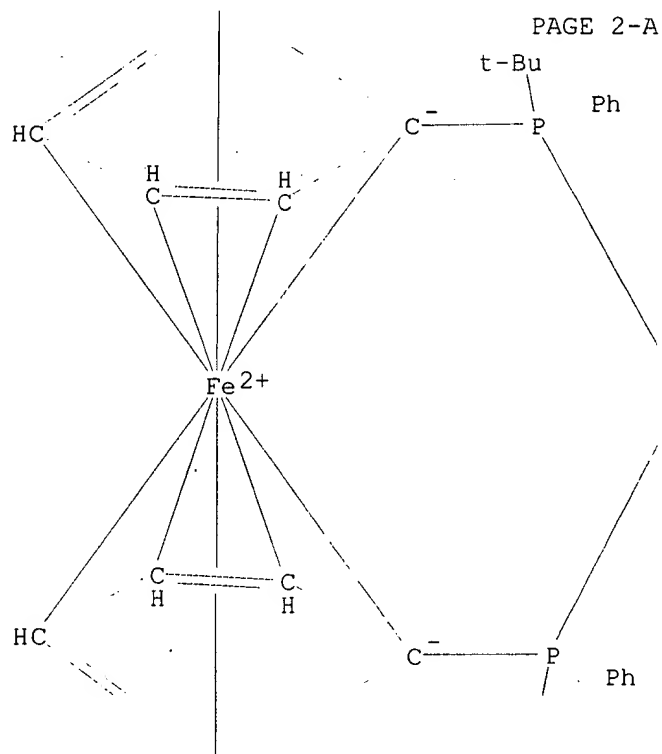
CM 1

CRN 92269-94-8

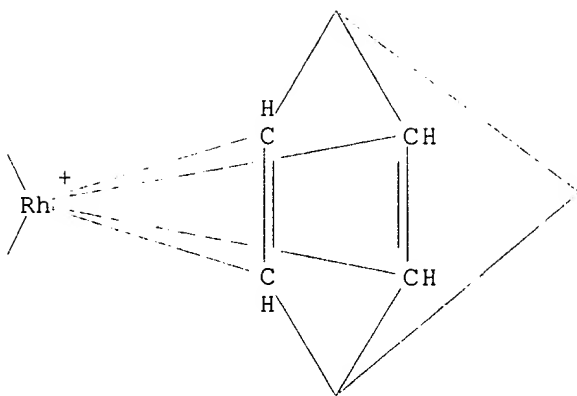
CMF C37 H44 Fe P2 Rh

CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

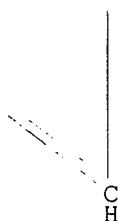


PAGE 2-B



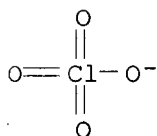
PAGE 3-A

t-Bu



CM 2

CRN 14797-73-0
CMF C1 O4



IT 92468-68-3P 92468-70-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)

RN 92468-68-3 HCAPLUS

CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-
P,P']tri-μ-hydrodihydrodi-, stereoisomer, perchlorate, compd. with
methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1
CMF C H4 O

H₃C--OH

CM 2

CRN 92468-67-2

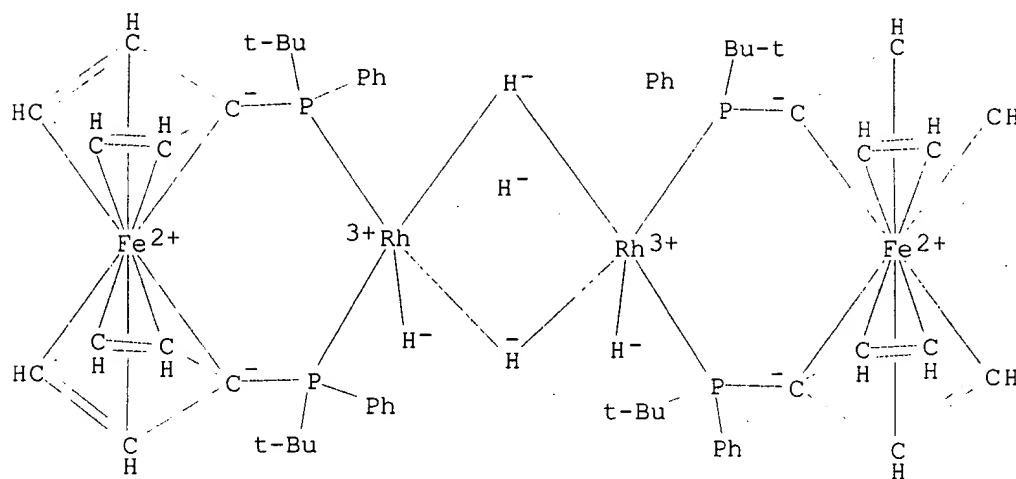
CMF C60 H77 Fe2 P4 Rh2 . Cl O4

CM 3

CRN 92468-66-1

CMF C60 H77 Fe2 P4 Rh2

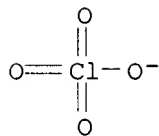
CCI CCS



CM 4

CRN 14797-73-0

CMF Cl O4



RN 92468-70-7 HCAPLUS

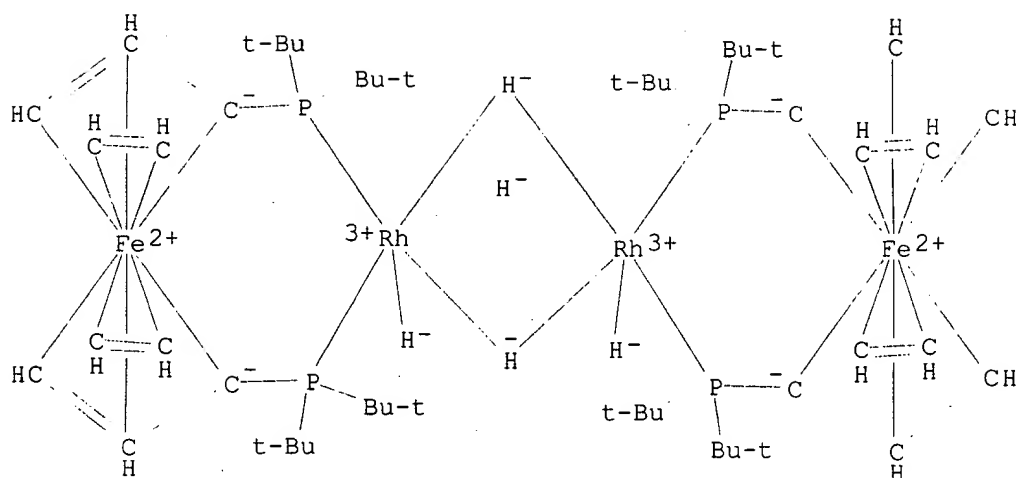
CN Rhodium(1+), bis[1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92468-69-4

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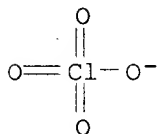
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



IT 92468-67-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

RN 92468-67-2 HCAPLUS

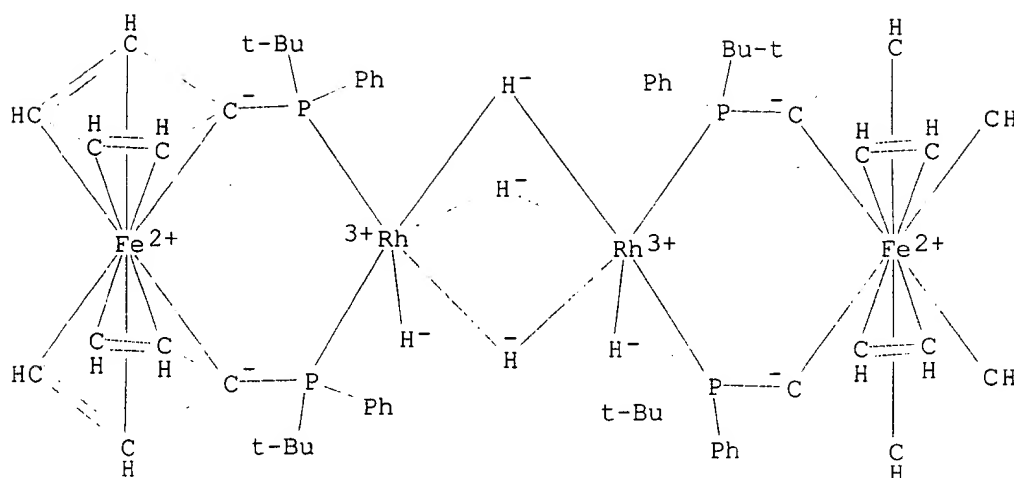
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-
P,P']tri- μ -hydrodihydrodi-, stereoisomer, perchlorate (9CI) (CA INDEX
NAME)

CM 1

CRN 92468-66-1

CMF C60 H77 Fe2 P4 Rh2

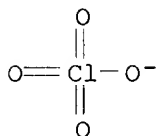
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



L104 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:215759 HCAPLUS

DN 98:215759

ED Entered STN: 12 May 1984

TI Structure of the **hydrogenation** catalyst [(PP)Rh(NBD)]ClO₄, PP = (η⁵-(Me₃C)₂PC₅H₄)₂Fe, and some comparative rate studies

AU Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones, Terry

CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SO Organometallics (1983), 2(6), 714-19

CODEN: ORGND7; ISSN: 0276-7333

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 34, 75

GI For diagram(s), see printed CA Issue.

AB In this abstract NBD is norbornadiene. The structure of the homogeneous **hydrogenation** precursor I (R = Me₃C).cntdot.Rh(NBD)ClO₄(II), determined crystallog., shows that Rh is in a distorted square planar environment involving both NBD double bonds; the bidentates atoms also chelate the Rh atom. The steric and electronic effects of the bis(phosphine) ligands in the ferrocenyl moiety are related to the relative **hydrogenation** kinetics of CH₂:CRCO₂H (R = NHAc, CH₂CO₂H) or PhCH:CRCO₂H (R = NHAc, Me) in EtOH or MeOH containing II or I (R = Ph).cntdot.Rh(NBD)ClO₄. The mechanism was discussed.

ST crystal structure **rhodium** phosphinoferrrocene complex; mol

- structure **rhodium** norbornadiene complex; **hydrogenation** catalyst **rhodium** complex; kinetics **hydrogenation** acetamidoacrylic acid; mechanism hydration catalyst acetamidoacrylic acid; acetamidocinnamic acid kinetics **hydrogenation**; itaconic acid kinetics **hydrogenation**; steric effect kinetics **hydrogenation**; solvent kinetics **hydrogenation**
- IT Ligands
RL: RCT (Reactant); RACT (Reactant or reagent).
(bis(phosphino)ferrocenes, for **rhodium** in homogeneous **hydrogenation** catalyst, substituent effects and)
- IT Bond
(in **rhodium** complex homogeneous **hydrogenation** catalyst containing bis(phosphino)ferrocene ligands)
- IT Kinetics of **hydrogenation**
(of alkenoic acids in presence of **rhodium** complexes containing bis(phosphino)ferrocenes)
- IT **Hydrogenation**
(of alkenoic acids, in presence of **rhodium** complexes containing bis(phosphino)ferrocenes, mechanism of)
- IT Crystal structure
Molecular structure
(of **rhodium** complex with bis(phosphino)ferrocene)
- IT Steric effect
Substituent effect
(on **hydrogenation** activity of **rhodium** complexes containing bis(phosphino)ferrocenes)
- IT Solvent effect
(on **hydrogenation** of alkenoic acids in presence of **rhodium** complexes with bis(phosphino)ferrocenes)
- IT **Hydrogenation catalysts**
(**rhodium** complexes containing norbornadiene and bis(phosphino)ferrocenes, for alkenoic acids, kinetics and mechanism with)
- IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd., **hydrogenation** of, in presence of **rhodium** complexes containing bis(phosphino)ferrocenes)
- IT 84680-96-6 84680-98-8
RL: CAT (Catalyst use); USES (Uses)
(**hydrogenation** catalyst, for alkenoic acids, kinetics and mechanism with)
- IT 97-65-4, reactions 1199-77-5 5429-56-1 5469-45-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, in presence of **rhodium** complexes with norbornadiene and bis(phosphino)ferrocenes, kinetics and mechanism of)
- IT 84680-95-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium** and norbornadiene)
- IT 11106-52-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorodibutylphosphine)
- IT 13716-10-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dilithioferrocenebis(tetramethylethylenediamine))
- IT 84680-96-6 84680-98-8
RL: CAT (Catalyst use); USES (Uses)
(**hydrogenation** catalyst, for alkenoic acids, kinetics and mechanism with)
- RN 84680-96-6 HCAPLUS
- CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

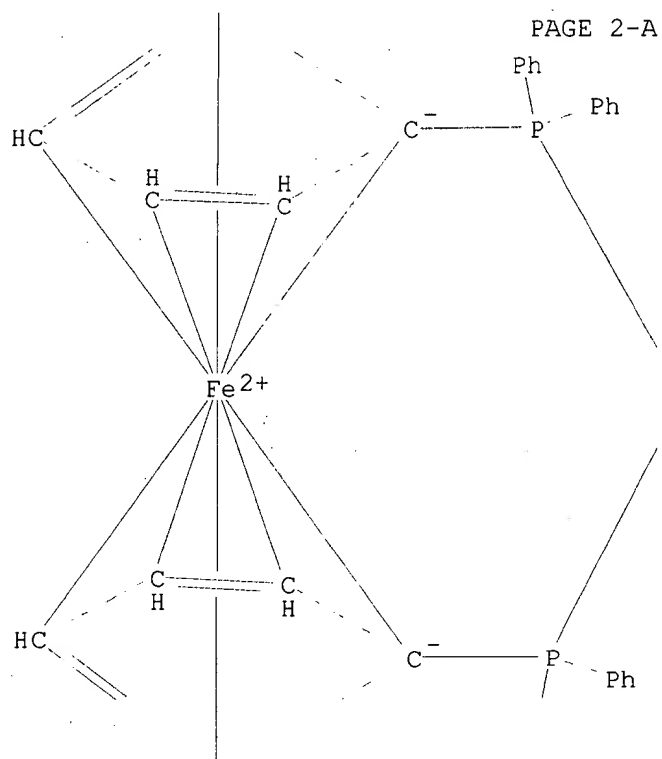
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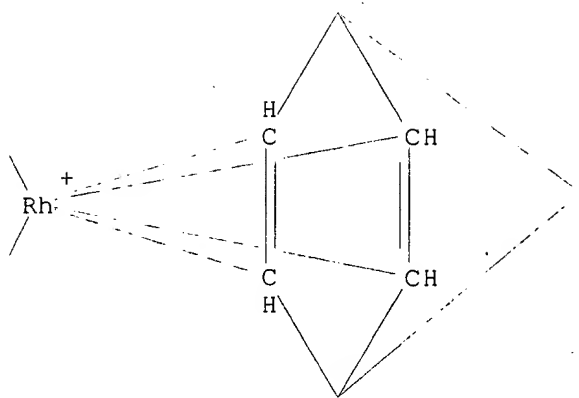
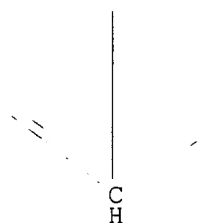
CMF C41 H36 Fe P2 Rh

CCI CCS

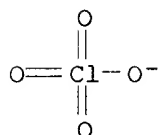
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B

PAGE 3-A
Ph

CM 2

CRN 14797-73-0
CMF C1 O4

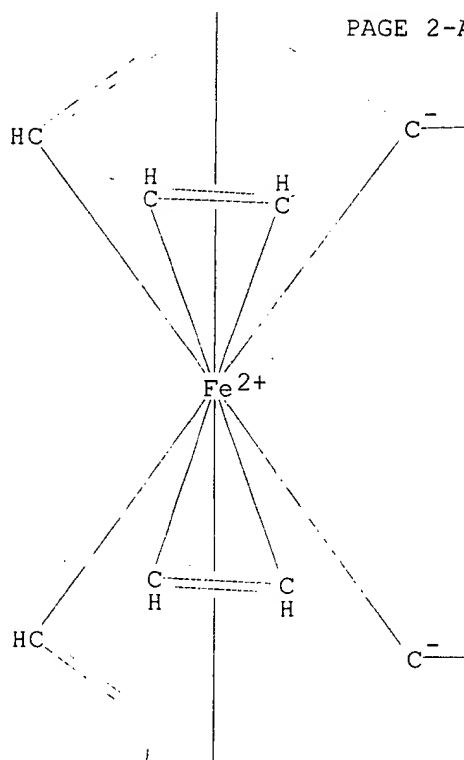
RN 84680-98-8 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI)
 (CA INDEX NAME)

CM 1

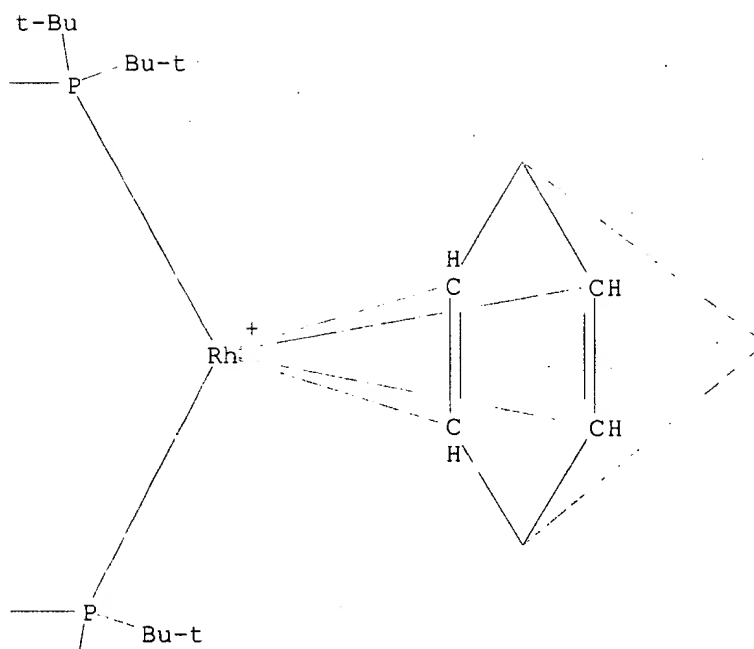
CRN 84680-97-7
CMF C33 H52 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A

$$\begin{array}{c} | \\ \text{C} \\ | \\ \text{H} \end{array}$$

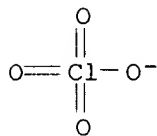
PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0

CMF Cl O4

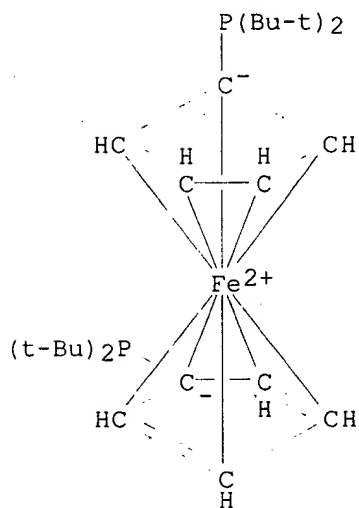


IT 84680-95-5P

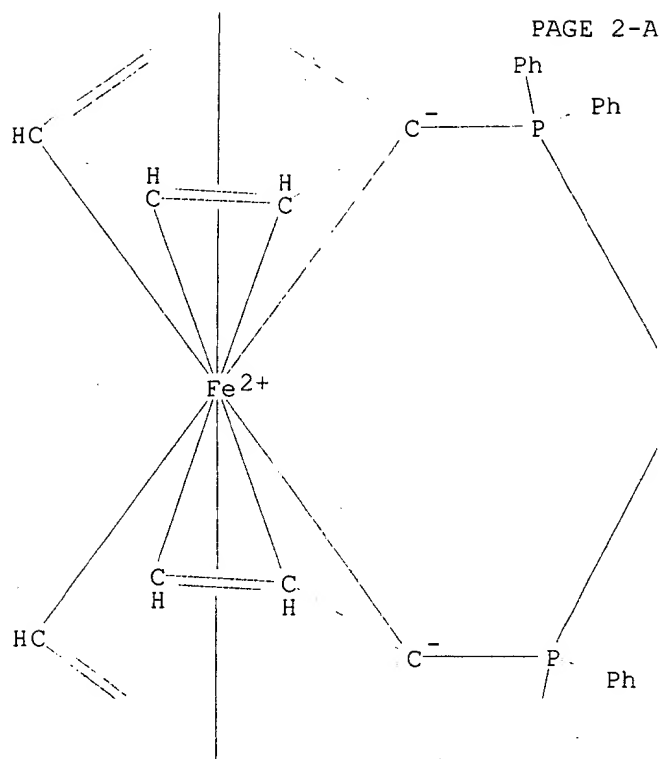
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with **rhodium** and norbornadiene)

RN 84680-95-5 HCAPLUS

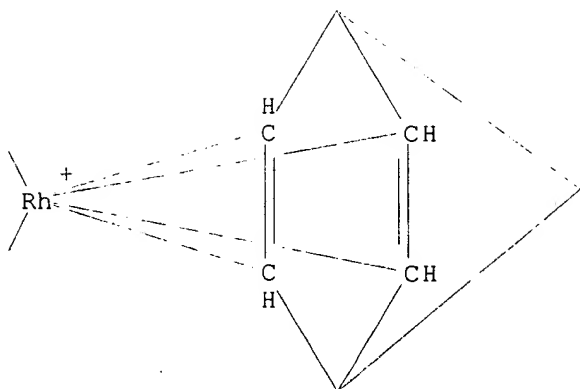
CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]- (9CI) (CA INDEX NAME)

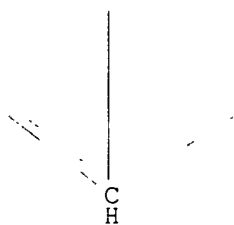


DN 95:210374
 ED Entered STN: 12 May 1984
 TI The mechanism of asymmetric homogeneous hydrogenation. Solvent complexes and dihydrides from rhodium diphosphine precursors
 AU Brown, John M.; Chaloner, Penny A.; Kent, Alexander G.; Murrer, Barry A.; Nicholson, Philip N.; Parker, David; Sidebottom, Philip J.
 CS Dyson Perrins Lab., Oxford, OX1 3QY, UK
 SO Journal of Organometallic Chemistry (1981), 216(2), 263-76
 CODEN: JORCAI; ISSN: 0022-328X
 DT Journal
 LA English
 CC 67-1 (Catalysis and Reaction Kinetics)
 Section cross-reference(s): 22
 AB Bicyclo[2.2.1]hepta-2,5-diene and cycloocta-1,5 diene(biphosphine)Rh tetrafluoroborates react with H at 1 atm in methanol or other polar solvents to give as initial product either a solvated dihydride or a solvate. Depending on phosphine structure the equilibrium between these 2 species varies widely. Dihydrides are normally the stable product when the ligand is a monophosphine although (o-methoxyphenyl)methylphenylphosphine is an exception. Cis Chelating biphosphines normally form solvate complexes with no affinity for H. R-Ph bis(diphenylphosphinoethane) falls into this category, but the 31P NMR spectra of its complexes demonstrate an equilibrium between monomeric and dimeric species, and addition of triethylamine gives rise to a trimer. Trans-Chelating biphosphines show more variable behavior, and in the case of bis-1,5-diphenylphosphinopentane, a number of complexes, including one requiring C-H activation, were observed
 ST hydrogenation catalyst rhodium phosphine olefin; bicycloheptadiene rhodium phosphine hydrogenation catalyst; cyclooctadiene rhodium phosphine hydrogenation catalyst
 IT Hydrogenation catalysts
 (rhodium bicycloheptadiene by phosphinetetrafluoroborates, solvent complexes and dihydrides of)
 IT 79790-95-7
 RL: CAT (Catalyst use); USES (Uses)
 (hydrogenation catalysts, preparation of solvent complexes and dihydrides of)
 IT 34664-30-7 34664-31-8 60430-43-5 60584-05-6 65606-90-8
 68811-61-0 68811-82-5 74498-00-3 75085-38-0 79255-71-3
 79790-89-9 79790-91-3 **79790-98-0** 79795-96-3
 RL: CAT (Catalyst use); USES (Uses)
 (hydrogenation catalysts, solvent complexes and dihydrides of)
 IT 69381-91-5P 121902-83-8P
 RL: PREP (Preparation)
 (preparation of)
 IT **79790-98-0**
 RL: CAT (Catalyst use); USES (Uses)
 (hydrogenation catalysts, solvent complexes and dihydrides of)
 RN 79790-98-0 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, tetrafluoroborate(1-) (9CI)
 (CA INDEX NAME)
 CM 1
 CRN 79790-97-9
 CMF C41 H36 Fe P2 Rh
 CCI CCS



PAGE 2-B





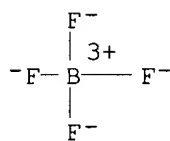
PAGE 3-A
Ph

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



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